

## ANGLE DISTORTION MODEL FOR PREDICTING ENEDIYNE ACTIVATION TOWARDS BERGMAN CYCLIZATION: AN ALTERNATE TO THE DISTANCE THEORY

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**1. Distance between alkyne carbon atoms a-b and c-d; angles  $P_a$ ,  $P_b$ ,  $D_c$  and  $D_d$  for the studied enediynes**

Entry	Enediyne Molecule (Along with their reactivities)	DFT Theory Level	a-b (distance in Å)	c-d (distance in Å)	Bond angle (in degrees)			
					$P_a$	$P_b$	$D_c$	$D_d$
A	10	B3LYP/6-31G+(d,p)	3.002	4.488	182.26	182.27	178.80	178.74
		B3LYP/6-311G++(d,p)	2.994	4.463	182.06	182.04	179.17	179.18
B	11	B3LYP/6-31G+(d,p)	2.813	4.171	183.62	183.62	178.13	178.13
		B3LYP/6-311G++(d,p)	2.809	4.152	183.39	183.39	178.46	178.46
C	12	B3LYP/6-31G+(d,p)	3.015	4.518	182.41	182.41	178.90	178.90
		B3LYP/6-311G++(d,p)	3.007	4.490	182.06	182.06	179.14	179.14
D	13	B3LYP/6-31G+(d,p)	2.713	2.918	156.80	156.51	169.65	169.89
		B3LYP/6-311G++(d,p)	2.696	2.930	157.55	157.52	168.80	168.82
E	14	B3LYP/6-31G+(d,p)	2.755	3.376	165.40	165.40	172.05	172.05
		B3LYP/6-311G++(d,p)	2.746	3.383	165.89	165.89	171.43	171.43
F	15	B3LYP/6-31G+(d,p)	2.748	3.353	166.90	166.90	172.81	172.81
		B3LYP/6-311G++(d,p)	2.739	3.357	167.34	167.34	172.29	172.29
G	16	B3LYP/6-31G+(d,p)	2.753	3.350	167.10	167.11	172.96	172.95
		B3LYP/6-311G++(d,p)	2.744	3.352	167.53	167.54	172.53	172.53
H	17	B3LYP/6-31G+(d,p)	2.834	3.763	171.88	170.56	172.24	169.24

		B3LYP/6-311G++(d,p)	2.829	3.748	171.76	170.29	172.47	169.56
<b>I</b>	<b>18</b>	B3LYP/6-31G+(d,p)	2.916	4.168	177.45	177.87	174.46	174.74
		B3LYP/6-311G++(d,p)	2.912	4.149	177.07	177.62	174.73	175.26
<b>J</b>	<b>19</b>	B3LYP/6-31G+(d,p)	2.738	3.339	164.24	166.38	171.71	172.18
		B3LYP/6-311G++(d,p)	2.729	3.338	164.72	166.53	171.30	172.02
<b>K</b>	<b>20</b>	B3LYP/6-31G+(d,p)	2.740	3.348	166.64	167.68	171.74	171.10
		B3LYP/6-311G++(d,p)	2.732	3.345	167.02	167.77	171.53	171.00
<b>L</b>	<b>21</b>	B3LYP/6-31G+(d,p)	2.746	3.298	163.81	164.23	175.00	174.88
		B3LYP/6-311G++(d,p)	2.734	3.310	164.54	164.97	174.08	174.12
<b>M</b>	<b>22</b>	B3LYP/6-31G+(d,p)	2.770	3.441	166.33	166.25	171.00	169.84
		B3LYP/6-311G++(d,p)	2.760	3.436	166.60	166.43	170.80	169.74
<b>N</b>	<b>23</b>	B3LYP/6-31G+(d,p)	2.773	3.482	167.01	167.01	168.31	168.66
		B3LYP/6-311G++(d,p)	2.764	3.470	167.10	167.05	168.39	168.81
<b>O</b>	<b>24</b>	B3LYP/6-31G+(d,p)	2.763	3.504	168.15	168.11	168.73	166.52
		B3LYP/6-311G++(d,p)	2.758	3.490	168.14	167.83	168.93	166.78
<b>P</b>	<b>25</b>	B3LYP/6-31G+(d,p)	2.715	3.171	161.92	162.59	172.92	175.43
		B3LYP/6-311G++(d,p)	2.702	3.182	162.68	163.41	172.83	174.97
<b>Q</b>	<b>26</b>	B3LYP/6-31G+(d,p)	2.812	3.654	170.17	168.98	161.45	163.00
		B3LYP/6-311G++(d,p)	2.807	3.628	169.46	168.69	162.46	163.58

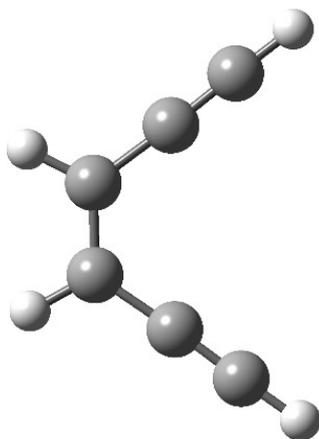
<b>R</b>	<b>27</b>	B3LYP/6-31G+(d,p)	2.746	3.300	163.21	164.90	172.73	173.54
		B3LYP/6-311G++(d,p)	2.733	3.309	163.87	165.60	172.38	172.75
<b>S</b>	<b>28</b>	B3LYP/6-31G+(d,p)	2.740	3.252	163.36	162.98	175.37	173.80
		B3LYP/6-311G++(d,p)	2.727	3.260	164.23	163.47	174.88	173.19
<b>T</b>	<b>29</b>	B3LYP/6-31G+(d,p)	2.748	3.418	168.62	164.93	172.52	170.90
		B3LYP/6-311G++(d,p)	2.740	3.414	168.71	165.29	172.39	170.59
<b>U</b>	<b>30</b>	B3LYP/6-31G+(d,p)	2.751	3.468	168.99	166.68	165.85	170.55
		B3LYP/6-311G++(d,p)	2.745	3.456	168.73	166.87	166.27	170.47
<b>V</b>	<b>31</b>	B3LYP/6-31G+(d,p)	2.750	3.434	167.53	166.67	168.52	170.78
		B3LYP/6-311G++(d,p)	2.742	3.429	167.58	166.93	168.56	170.50
<b>W</b>	<b>32</b>	B3LYP/6-31G+(d,p)	2.748	3.420	167.17	166.49	169.36	171.28
		B3LYP/6-311G++(d,p)	2.741	3.416	167.22	166.73	169.29	171.08
<b>X</b>	<b>33</b>	B3LYP/6-31G+(d,p)	2.733	3.315	165.33	164.73	172.93	173.86
		B3LYP/6-311G++(d,p)	2.722	3.317	165.62	165.29	172.66	173.28

## 2. Optimized geometries, cartesian coordinates of the optimized structures and energy values (in atomic units)

**ENTRY: A**

**MOLECULE: 10**

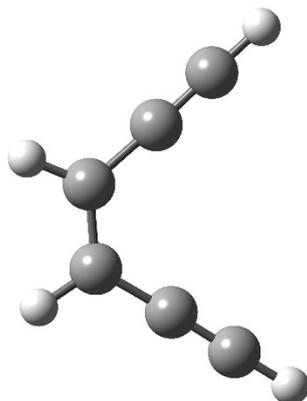
<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-230.901361



Cartesian coordinates of optimized enediyne **10** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	-1.14885800	0.55569700	0.00000000
C	0.00000000	1.27617700	0.00000000
C	1.31051500	0.73524900	0.00000000
C	-1.23260200	-0.85961300	0.00000000
C	-1.35198900	-2.06743600	0.00000000
C	2.44990900	0.31706200	0.00000000
H	-1.43456200	-3.13035900	0.00000000
H	3.44243100	-0.07219300	0.00000000
H	-2.09181200	1.09838100	0.00000000
H	-0.07790500	2.36135300	0.00000000

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-230.951199

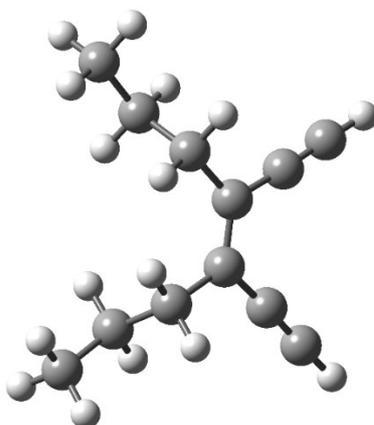


Cartesian coordinates of optimized enediyne **10** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	0.00000000	1.27253200	0.00000000
C	-1.14526200	0.55486100	0.00000000
C	-1.22920200	-0.85732900	0.00000000
C	1.30743900	0.73225700	0.00000000
C	2.43786400	0.31209800	0.00000000
C	-1.34365800	-2.05785300	0.00000000
H	3.42840900	-0.07256400	0.00000000
H	-1.42933700	-3.11700800	0.00000000
H	-0.07436500	2.35593400	0.00000000
H	-2.08778300	1.09424100	0.00000000

**ENTRY: B**  
**MOLECULE: 11**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-466.810397



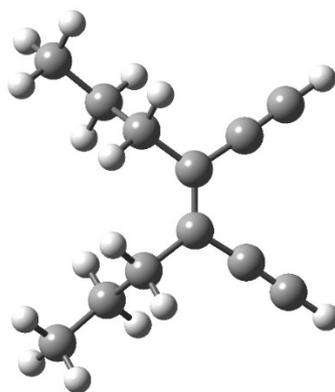
Cartesian coordinates of optimized enediyne **11** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

```

C      -0.68406100  0.67309100  0.35788000
C      0.68428100  0.67306000  0.35783500
C      1.40679500  1.85275700  0.00225400
C     -1.40647700  1.85282700  0.00228100
C     -2.08513000  2.81784500 -0.28307400
C      2.08546900  2.81777500 -0.28305700
C      1.55361100 -0.52474800  0.69945400
C      2.19206100 -1.18877300 -0.53862800
C      3.12290200 -2.34770600 -0.16586900
C     -1.55343400 -0.52474700  0.69949000
C     -2.19208600 -1.18858500 -0.53861100
C     -3.12367800 -2.34691600 -0.16584200
H     -2.65193100  3.68362300 -0.53906100
H      2.65235500  3.68348700 -0.53908800
H      2.35460900 -0.18668100  1.36926800
H      0.97790900 -1.27276800  1.25146700
H      1.39585700 -1.54863100 -1.20255900
H      2.74911100 -0.43218300 -1.10384100
H      3.55951500 -2.80676900 -1.05922600
H      3.94789700 -2.00423100  0.46920500
H      2.58608400 -3.13133000  0.38229200
H     -0.97770300 -1.27289900  1.25133700
H     -2.35427200 -0.18664800  1.36946300
H     -2.74856400 -0.43173300 -1.10403900
H     -1.39594200 -1.54905000 -1.20227800
H     -3.56024100 -2.80602400 -1.05919900
H     -2.58748900 -3.13066500  0.38275800
H     -3.94871200 -2.00278700  0.46882700

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<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-466.901875

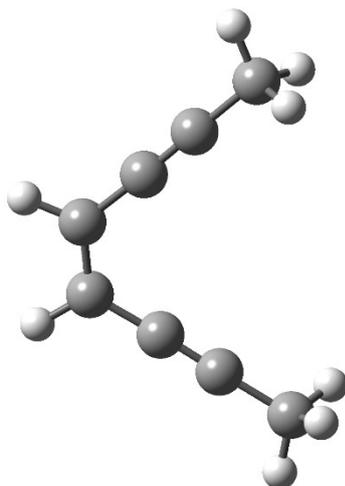


Cartesian coordinates of optimized enediyne **11** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	-0.68178100	0.67113000	0.35849700
C	0.68178200	0.67112800	0.35849900
C	1.40425400	1.84706100	0.00207000
C	-1.40425100	1.84706300	0.00206500
C	-2.07591900	2.80771600	-0.28302900
C	2.07593100	2.80770700	-0.28302500
C	1.55026200	-0.52507500	0.69976500
C	2.19279500	-1.18264900	-0.53765800
C	3.12470200	-2.33935200	-0.16715200
C	-1.55026600	-0.52507100	0.69976200
C	-2.19279800	-1.18264400	-0.53766200
C	-3.12471700	-2.33933800	-0.16715600
H	-2.64348500	3.66864800	-0.53866000
H	2.64357800	3.66855600	-0.53875500
H	2.34705800	-0.18731500	1.37159900
H	0.97544200	-1.27397800	1.24760700
H	1.40053300	-1.54126300	-1.20369100
H	2.74782900	-0.42392500	-1.09800300
H	3.56343100	-2.79373300	-1.05953300
H	3.94632600	-1.99663600	0.46939200
H	2.58978400	-3.12482200	0.37641700
H	-0.97544900	-1.27397400	1.24760700
H	-2.34706200	-0.18730700	1.37159500
H	-2.74782300	-0.42391700	-1.09801100
H	-1.40053600	-1.54126600	-1.20368900
H	-3.56343700	-2.79372400	-1.05953800
H	-2.58981000	-3.12480600	0.37642700
H	-3.94634700	-1.99661000	0.46937400

**ENTRY: C**  
**MOLECULE: 12**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-309.560134



Cartesian coordinates of optimized enediyne **12** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	-0.67905800	1.74879700	-0.00011900
C	0.67906400	1.74881000	0.00011400
C	1.50772800	0.59819900	0.00023400
C	-1.50768500	0.59817100	-0.00019800
C	-2.25920500	-0.35781700	-0.00027800
C	2.25923800	-0.35779800	0.00033200
C	-3.13885000	-1.52207900	0.00018000
C	3.13880400	-1.52212300	-0.00021000
H	-1.18455400	2.71277800	-0.00025000
H	1.18453200	2.71280700	0.00009000
H	-2.96486400	-2.14681100	-0.88365700
H	-2.96669800	-2.14470700	0.88585900
H	-4.19303200	-1.22366500	-0.00126800
H	4.19300800	-1.22377900	-0.00088800
H	2.96626400	-2.14580800	0.88465300
H	2.96512900	-2.14577500	-0.88486700

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-309.622878

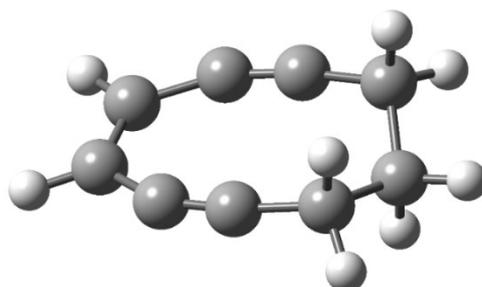


Cartesian coordinates of optimized enediyne **12** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	-0.67663500	1.74529300	-0.00004700
C	0.67666400	1.74530400	0.00000300
C	1.50365200	0.59765500	0.00005100
C	-1.50360400	0.59763000	-0.00007400
C	-2.24506300	-0.35692000	-0.00007800
C	2.24510900	-0.35689700	0.00011200
C	-3.12055700	-1.51947100	-0.00000800
C	3.12048300	-1.51954000	0.00003000
H	-1.18292100	2.70669100	-0.00006600
H	1.18293600	2.70671000	0.00003100
H	-2.94573800	-2.14203500	-0.88300300
H	-2.94690100	-2.14105400	0.88391000
H	-4.17331100	-1.22263500	-0.00085800
H	4.17326700	-1.22281100	-0.00111800
H	2.94699900	-2.14104100	0.88404000
H	2.94536700	-2.14215000	-0.88287400

**ENTRY: D**  
**MOLECULE: 13**

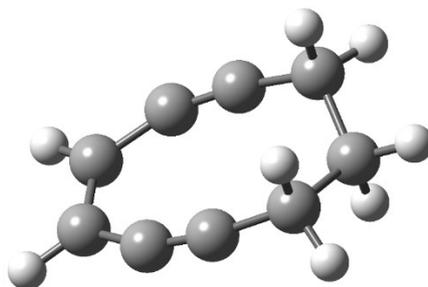
<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-347.643796



Cartesian coordinates of optimized enediyne **13** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	-2.31011200	-0.68665900	0.06187300
C	-2.31228300	0.68315700	0.06206200
C	-1.05807800	-1.35598700	-0.01670600
C	-1.06232900	1.35660100	-0.01631800
C	0.15441500	-1.45965200	-0.09310500
C	0.15042700	1.45809900	-0.09352300
C	1.60851900	-1.32005500	-0.19256800
C	1.60470600	1.32215100	-0.19291300
C	2.12054600	0.00161400	0.44571800
H	-3.24461200	-1.23603600	0.11910000
H	-3.24855600	1.22948400	0.11954600
H	2.11726500	-2.16066900	0.29584600
H	1.90752600	-1.35479200	-1.25087400
H	1.90421700	1.35746700	-1.25099700
H	2.11116700	2.16392900	0.29593400
H	1.86271500	0.00156900	1.51021800
H	3.21542400	0.00342500	0.37410900

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-347.712884



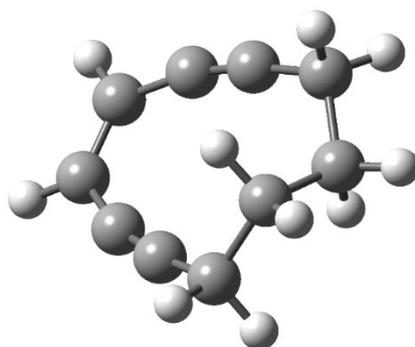
Cartesian coordinates of optimized enediyne **13** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	-2.30275900	-0.68259000	0.06163100
C	-2.30291100	0.68237900	0.06173400
C	-1.05284400	-1.34820600	-0.01618000
C	-1.05311400	1.34827700	-0.01599600
C	0.15043000	-1.46516100	-0.09257500
C	0.15016100	1.46497400	-0.09285600
C	1.60036700	-1.32121700	-0.19283700
C	1.60014900	1.32133800	-0.19284900
C	2.11071000	0.00013700	0.44486800
H	-3.23562700	-1.23118100	0.11773000
H	-3.23590100	1.23074700	0.11793800

H	2.11038500	-2.15911900	0.29471500
H	1.89759500	-1.35648400	-1.24962000
H	1.89757300	1.35675700	-1.24957600
H	2.10980400	2.15940200	0.29481200
H	1.85112200	0.00008600	1.50693800
H	3.20391700	0.00020300	0.37742700

**ENTRY: E**  
**MOLECULE: 14**

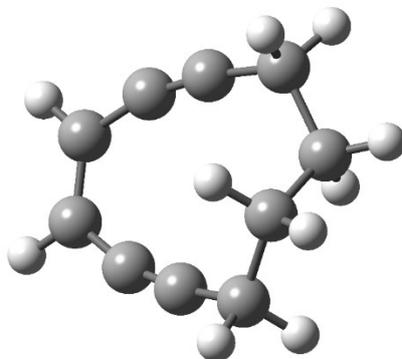
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<b>Energy (Hartree)</b>	-386.969326



Cartesian coordinates of optimized enediyne **14** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	0.01455200	0.68206800	2.56791300
C	-0.01455200	-0.68206800	2.56791300
C	0.01467300	1.37758600	1.32946500
C	-0.01467300	-1.37758600	1.32946500
C	-0.01455200	1.68815700	0.15276500
C	0.01455200	-1.68815700	0.15276500
C	-0.11780500	1.87332000	-1.29416600
C	-0.52948500	0.56780200	-2.02946600
C	0.11780500	-1.87332000	-1.29416600
C	0.52948500	-0.56780200	-2.02946600
H	0.02826000	1.22881600	3.50646000
H	-0.02826000	-1.22881600	3.50646000
H	-0.85977000	2.65203000	-1.51493700
H	0.83603300	2.24061900	-1.69814700
H	-1.46616300	0.20899000	-1.58757700
H	-0.76105800	0.84436200	-3.06487000
H	0.85977000	-2.65203000	-1.51493700
H	-0.83603300	-2.24061900	-1.69814700
H	1.46616300	-0.20899000	-1.58757700
H	0.76105800	-0.84436200	-3.06487000

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-387.045722

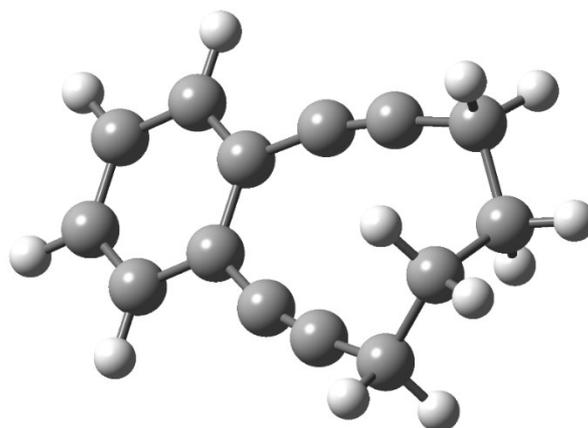


Cartesian coordinates of optimized enediyne **14** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	0.01525000	0.67956600	2.55553400
C	-0.01525000	-0.67956600	2.55553400
C	0.01525000	1.37305600	1.32004000
C	-0.01525000	-1.37305600	1.32004000
C	-0.01409800	1.69150700	0.15336200
C	0.01409800	-1.69150700	0.15336200
C	-0.12263800	1.87334800	-1.28970100
C	-0.53189400	0.56457900	-2.01722800
C	0.12263800	-1.87334800	-1.28970100
C	0.53189400	-0.56457900	-2.01722800
H	0.02943500	1.22609600	3.49206500
H	-0.02943500	-1.22609600	3.49206500
H	-0.86745800	2.64717700	-1.50851500
H	0.82657200	2.24311300	-1.69707100
H	-1.46164100	0.20371000	-1.56776800
H	-0.77167500	0.83252800	-3.05074600
H	0.86745800	-2.64717700	-1.50851500
H	-0.82657200	-2.24311300	-1.69707100
H	1.46164100	-0.20371000	-1.56776800
H	0.77167500	-0.83252800	-3.05074600

**ENTRY: F**  
**MOLECULE: 15**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-540.635643



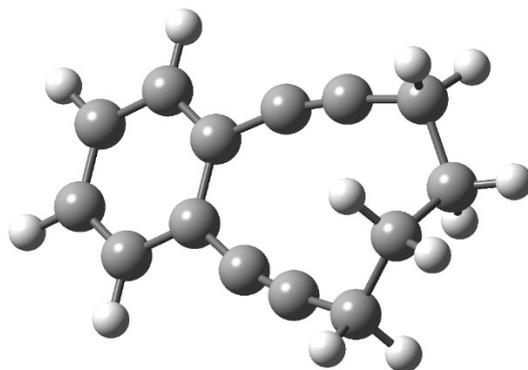
Cartesian coordinates of optimized enediyne **15** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

```

C      0.00547600  0.71554800  1.35808400
C     -0.00547600 -0.71554800  1.35808400
C     -0.00547600  1.37386200  0.09092100
C      0.00547600 -1.37386200  0.09092100
C     -0.04149000  1.67606800 -1.08556900
C      0.04149000 -1.67606800 -1.08556900
C     -0.13490800  1.86606800 -2.53268900
C     -0.53328900  0.56387000 -3.27966900
C      0.13490800 -1.86606800 -2.53268900
C      0.53328900 -0.56387000 -3.27966900
C      0.01432100  1.40031900  2.58300200
C      0.00806900  0.69940100  3.78921600
C     -0.00806900 -0.69940100  3.78921600
C     -0.01432100 -1.40031900  2.58300200
H     -0.87858100  2.64253200 -2.75532800
H      0.82083100  2.23898600 -2.92672200
H     -0.75780900  0.84706500 -4.31481100
H     -1.47153000  0.19510700 -2.84928500
H      0.87858100 -2.64253200 -2.75532800
H     -0.82083100 -2.23898600 -2.92672200
H      0.75780900 -0.84706500 -4.31481100
H      1.47153000 -0.19510700 -2.84928500
H      0.02439300  2.48559500  2.57782800
H      0.01453900  1.24427900  4.72854700
H     -0.01453900 -1.24427900  4.72854700
H     -0.02439300 -2.48559500  2.57782800

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<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-540.738401



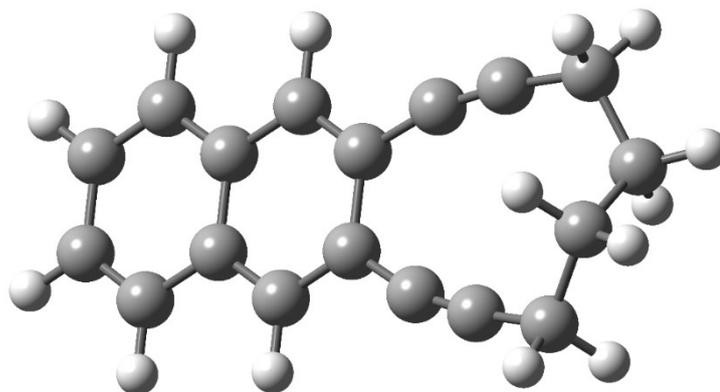
Cartesian coordinates of optimized enediyne **15** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	0.00579200	0.71387500	1.35068200
C	-0.00579200	-0.71387500	1.35068200
C	-0.00579200	1.36950200	0.08581400
C	0.00579200	-1.36950200	0.08581400
C	-0.04338200	1.67793000	-1.08145100
C	0.04338200	-1.67793000	-1.08145100
C	-0.14571900	1.86568900	-2.52440200
C	-0.53793600	0.55841700	-3.26258700
C	0.14571900	-1.86568900	-2.52440200
C	0.53793600	-0.55841700	-3.26258700
C	0.01512400	1.39684600	2.57296600
C	0.00841600	0.69757900	3.77612900
C	-0.00841600	-0.69757900	3.77612900
C	-0.01512400	-1.39684600	2.57296600
H	-0.89595300	2.63424700	-2.74293500
H	0.80301000	2.24508700	-2.92376100
H	-0.77352300	0.83111800	-4.29583100
H	-1.46709200	0.18442300	-2.82258600
H	0.89595300	-2.63424700	-2.74293500
H	-0.80301000	-2.24508700	-2.92376100
H	0.77352300	-0.83111800	-4.29583100
H	1.46709200	-0.18442300	-2.82258600
H	0.02589400	2.48018600	2.56821800
H	0.01528300	1.24111400	4.71399000
H	-0.01528300	-1.24111400	4.71399000
H	-0.02589400	-2.48018600	2.56821800

**ENTRY: G**  
**MOLECULE: 16**

DFT Theory Level	B3LYP/6-31G+(d,p)
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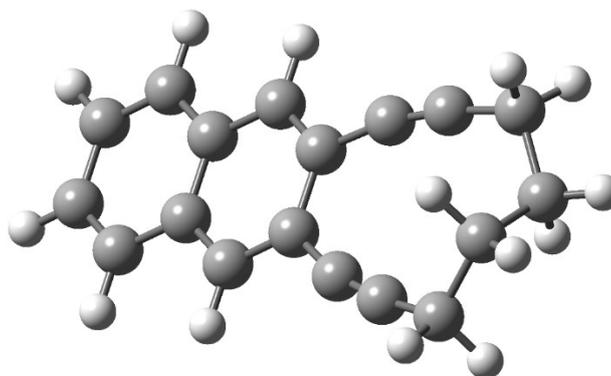
Energy (Hartree)	-694.287080
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Cartesian coordinates of optimized enediyne **16** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	0.12786200	-0.72589600	0.03628500
C	0.12785300	0.72586600	-0.03636700
C	-1.14335600	-1.37549300	0.05297700
C	-1.14338700	1.37542200	-0.05308800
C	-2.32104400	-1.67441200	0.03803100
C	-2.32104200	1.67445200	-0.03798300
C	-3.76804700	-1.86934100	-0.04507600
C	-4.51662700	-0.58883700	-0.50555500
C	-3.76804000	1.86935800	0.04518700
C	-4.51664900	0.58882800	0.50550500
C	1.33300000	-1.40369400	0.07323900
C	2.57437300	-0.71604400	0.03835600
C	2.57436500	0.71604600	-0.03839300
C	1.33298500	1.40368300	-0.07326400
C	3.81898000	-1.40215000	0.07510600
C	5.00994400	-0.70784300	0.03800200
C	5.00993700	0.70787000	-0.03797700
C	3.81896700	1.40216600	-0.07507000
H	-3.99024600	-2.68164300	-0.74959300
H	-4.16128900	-2.19513800	0.92807400
H	-5.55169800	-0.88367100	-0.71488200
H	-4.08797300	-0.26554400	-1.46122900
H	-3.99028500	2.68155600	0.74981300
H	-4.16128600	2.19532300	-0.92791100
H	-5.55172800	0.88369700	0.71475800
H	-4.08809800	0.26548300	1.46120600
H	1.33065600	-2.48840200	0.12803700
H	1.33062800	2.48839200	-0.12803300
H	3.81680400	-2.48757500	0.13299400
H	5.95364700	-1.24465500	0.06697800
H	5.95363300	1.24469800	-0.06683300
H	3.81678100	2.48759700	-0.13286500

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-694.416454



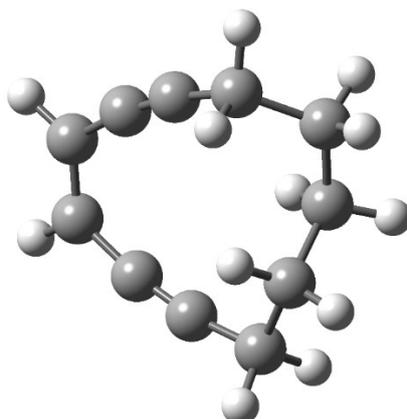
Cartesian coordinates of optimized enediyne **16** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	-0.12461500	-0.72454000	-0.03729800
C	-0.12461300	0.72453200	0.03732200
C	1.14456100	-1.37094200	-0.05399700
C	1.14456500	1.37093200	0.05403100
C	2.31325900	-1.67548900	-0.03820800
C	2.31325600	1.67549700	0.03813400
C	3.75621100	-1.86902700	0.05008200
C	4.49846400	-0.58579300	0.50794500
C	3.75621300	1.86902800	-0.05009700
C	4.49848600	0.58579300	-0.50792500
C	-1.32664500	-1.40044700	-0.07551000
C	-2.56595800	-0.71438000	-0.03961400
C	-2.56595600	0.71438000	0.03961800
C	-1.32664100	1.40044300	0.07552700
C	-3.80849100	-1.39895800	-0.07767000
C	-4.99578600	-0.70627700	-0.03935700
C	-4.99578400	0.70628500	0.03934200
C	-3.80848700	1.39896100	0.07766500
H	3.97581700	-2.67669800	0.75774900
H	4.15230800	-2.19802000	-0.91865100
H	5.53175500	-0.87331700	0.72496700
H	4.06339900	-0.25993500	1.45737900
H	3.97586000	2.67669800	-0.75775300
H	4.15226100	2.19802000	0.91865600
H	5.53178700	0.87331800	-0.72490000
H	4.06346700	0.25993400	-1.45737900
H	-1.32434600	-2.48314100	-0.13195500
H	-1.32433900	2.48313700	0.13197500
H	-3.80689900	-2.48233800	-0.13742000

H	-5.93821200	-1.24139600	-0.06919900
H	-5.93820800	1.24140600	0.06917700
H	-3.80689200	2.48234200	0.13741500

**ENTRY: H**  
**MOLECULE: 17**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-426.292154



Cartesian coordinates of optimized enediyne **17** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	-2.52644200	-1.16281400	0.11087300
C	-1.19297000	-1.61081000	-0.08454700
C	-0.00968200	-1.82807900	-0.27001300
C	1.43215800	-1.89335500	-0.51397700
C	2.27666600	-1.02466900	0.46467500
C	1.71900100	0.37823200	0.76028300
C	1.57263700	1.32078700	-0.44909500
C	0.51281600	2.43334400	-0.21954500
C	-0.81922700	1.84184900	-0.07017500
C	-1.81464900	1.15120600	0.04675500
C	-2.82816100	0.16493900	0.17097500
H	-3.32261800	-1.89606500	0.21134000
H	1.61339400	-1.56588300	-1.54678400
H	1.78753300	-2.92994600	-0.46303800
H	3.29261200	-0.96143800	0.05301200
H	2.35921600	-1.56134900	1.41735300
H	2.36270100	0.85419100	1.51197600
H	0.73763200	0.25482800	1.22932700
H	1.27018000	0.75851700	-1.33943200
H	2.53491900	1.79369500	-0.68390800
H	0.52390200	3.13723800	-1.06148700
H	0.76748100	3.01953000	0.67491900
H	-3.85983800	0.47290300	0.31946800

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-426.375595

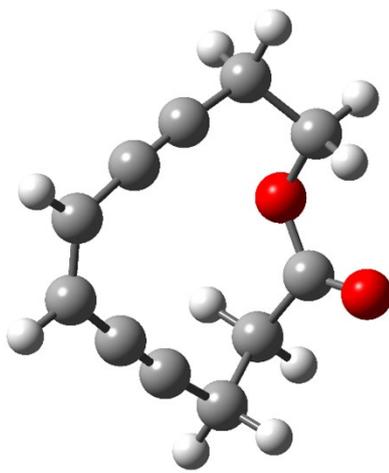
Cartesian coordinates of optimized enediyne **17** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	-2.51540400	-1.16366300	0.11169600
C	-1.18441400	-1.60860200	-0.08299400
C	-0.00795500	-1.82060200	-0.26921100
C	1.42956600	-1.88651800	-0.51409900
C	2.27525700	-1.01922400	0.46230300
C	1.71671500	0.38101800	0.75986700
C	1.56625900	1.32170400	-0.44855600
C	0.50248400	2.42802400	-0.21886600
C	-0.82281200	1.83182200	-0.07024200
C	-1.81263600	1.14628000	0.04599000
C	-2.81979900	0.15848000	0.17087100
H	-3.30787000	-1.89810900	0.21256900
H	1.60959700	-1.56077000	-1.54564600
H	1.78243400	-2.92190000	-0.46315700
H	3.28853900	-0.95365000	0.04973300
H	2.36132000	-1.55585800	1.41241900
H	2.36029900	0.85716700	1.50855200
H	0.73875400	0.25685200	1.23162200
H	1.26618000	0.75884800	-1.33686600
H	2.52501600	1.79675900	-0.68371900
H	0.50948200	3.13086600	-1.05921500
H	0.75318900	3.01416300	0.67435900
H	-3.85050300	0.46331700	0.31879700

**ENTRY: I**

**MOLECULE: 18**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-575.553081



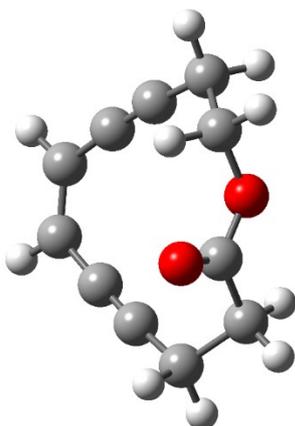
Cartesian coordinates of optimized enediyne **18** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

```

C      -3.11377700  0.08209200  0.13978400
C      -2.82866100 -1.24713100  0.16091800
C      -2.12281900  1.08644400 -0.00279100
C      -1.51346600 -1.76514200  0.04822200
C      -1.23693100  1.90842900 -0.13462600
C      -0.36945500 -2.16764100 -0.04216900
C      -0.08223900  2.78840100 -0.30760700
C      1.21801900  2.15486900  0.20519200
C      1.04536100 -2.52338300 -0.14830000
C      1.89695900 -1.38070400 -0.75675100
C      1.87250000 -0.15039600  0.13100800
O      1.45554400  0.94483300 -0.54547000
O      2.18147800 -0.15047100  1.30499500
H     -4.15031300  0.39680800  0.23557400
H     -3.64639000 -1.95526600  0.27392200
H      0.03217300  3.04321600 -1.36943500
H     -0.23099900  3.73532800  0.22829700
H      2.06266900  2.83025800  0.03520400
H      1.15943800  1.91181500  1.26732500
H      1.43742700 -2.76483600  0.84721300
H      1.16661700 -3.42118700 -0.76643900
H      1.54339100 -1.12672700 -1.75778900
H      2.93686800 -1.71932500 -0.82735300

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<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-575.678879



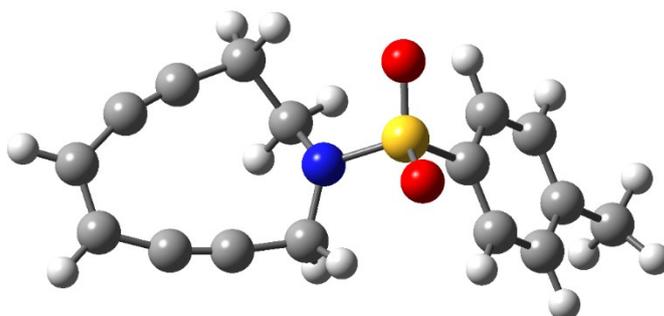
Cartesian coordinates of optimized enediyne **18** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	-3.10900400	0.04206800	0.14107800
C	-2.80547800	-1.27809900	0.16385100
C	-2.13681800	1.05983700	-0.00212200
C	-1.48711100	-1.77861700	0.05100100
C	-1.26427200	1.88517700	-0.13458100
C	-0.34337300	-2.15954400	-0.03862200
C	-0.12527900	2.77917800	-0.30678900
C	1.18136300	2.16332100	0.20560700
C	1.07035800	-2.50323700	-0.14523000
C	1.91209600	-1.35712600	-0.75674500
C	1.88098900	-0.12704100	0.12904000
O	1.43160300	0.95575300	-0.54335500
O	2.20740900	-0.11723100	1.29025800
H	-4.14798700	0.34167400	0.23701400
H	-3.61094100	-1.99712900	0.27790400
H	-0.01490900	3.03521800	-1.36677900
H	-0.28886600	3.72169400	0.22869900
H	2.01699500	2.84724100	0.03749200
H	1.12476900	1.92163700	1.26624200
H	1.46407600	-2.73971100	0.84883200
H	1.19606900	-3.40082300	-0.75945000
H	1.55489100	-1.10744900	-1.75535300
H	2.95297700	-1.68603600	-0.82874800

**ENTRY: J**

**MOLECULE: 19**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-1221.957159



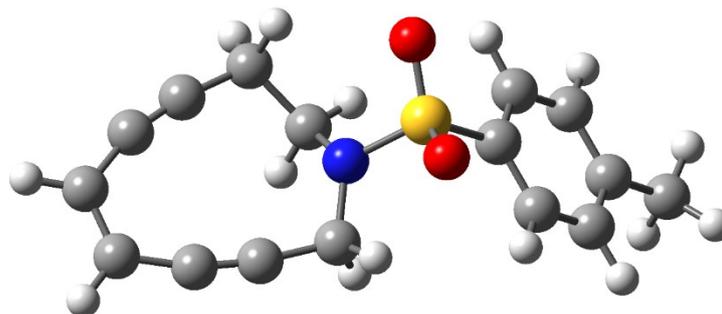
Cartesian coordinates of optimized enediyne **19** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

```

C      -5.44106900  -0.17326200  -0.62434800
C      -5.05235700  -1.46973500  -0.45266800
C      -4.45083400   0.84310900  -0.66996400
C      -3.67000200  -1.75455300  -0.29561000
C      -3.39747700   1.45261900  -0.67814700
C      -2.46205200  -1.71108700  -0.16405700
C      -2.04319500   1.99649100  -0.72395700
C      -0.97913600   0.89201800  -0.95975200
C      -1.03201100  -1.46165700   0.01261200
N      -0.76922900  -0.01207600   0.18951100
C       2.02575900   0.12734200   0.48503300
C       2.58835000  -1.15316100   0.51996700
C       3.80340100  -1.38143700  -0.12329800
C       4.47356600  -0.35041000  -0.80265100
C       3.89571800   0.92707800  -0.80747500
C       2.67856500   1.17464800  -0.16920900
C       5.77858800  -0.61808700  -1.51365300
S       0.43971400   0.42242300   1.28555200
O       0.33710500  -0.51311600   2.41000900
O       0.31060400   1.87375900   1.45934400
H      -6.49353600   0.07291200  -0.73039400
H      -5.78642400  -2.26914400  -0.42393000
H      -1.95507000   2.72398900  -1.54261600
H      -1.79841500   2.52931800   0.20116100
H      -1.27925100   0.27226900  -1.80924500
H      -0.03541100   1.37865100  -1.23181600
H      -0.67561800  -1.96645600   0.91437300
H      -0.46322900  -1.85861800  -0.84302000
H       2.09761400  -1.94836600   1.07085600
H       4.24585200  -2.37351600  -0.08474900
H       4.40880500   1.74541000  -1.30559600
H       2.25420500   2.17239000  -0.14710800
H       6.41377400  -1.29916500  -0.93866500
H       5.60170400  -1.08444200  -2.49085000
H       6.33763300   0.30589100  -1.68558000

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<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-1222.152364

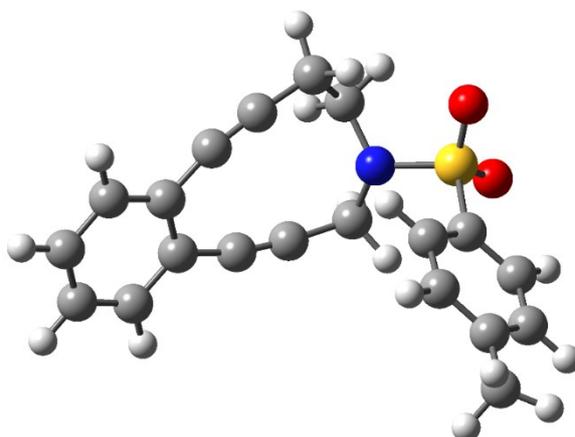


Cartesian coordinates of optimized enediyne **19** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	-5.42732600	-0.12941200	-0.61427000
C	-5.05328300	-1.42898000	-0.47493500
C	-4.42852100	0.87392500	-0.64195000
C	-3.67673300	-1.73089300	-0.33215900
C	-3.37991900	1.47646700	-0.64404000
C	-2.47523800	-1.70633600	-0.20601200
C	-2.02427400	2.00628500	-0.68928700
C	-0.97382500	0.89681500	-0.95107200
C	-1.04570800	-1.47604100	-0.03023600
N	-0.76603300	-0.03405600	0.17593500
C	2.02386200	0.11051900	0.48637300
C	2.58752300	-1.16618900	0.48117200
C	3.80342400	-1.36948100	-0.16133300
C	4.47317800	-0.31668400	-0.79952000
C	3.89528500	0.95629900	-0.76252900
C	2.67700400	1.17888100	-0.12441800
C	5.78087900	-0.55732300	-1.51144100
S	0.43188400	0.37456300	1.28843600
O	0.33004600	-0.58864100	2.38032300
O	0.29673500	1.81348700	1.50140400
H	-6.47561000	0.13079900	-0.70869300
H	-5.79409200	-2.21995500	-0.46059900
H	-1.93536000	2.74492500	-1.49536600
H	-1.76983000	2.52135800	0.24090000
H	-1.28377500	0.29944400	-1.81055000
H	-0.02712200	1.37636100	-1.21835900
H	-0.69398200	-2.00399300	0.85796800
H	-0.48526800	-1.86072700	-0.89405700
H	2.09679700	-1.97918700	1.00161800
H	4.24726400	-2.35956500	-0.15426600
H	4.40946700	1.79099500	-1.22706700
H	2.25179500	2.17290100	-0.06883400
H	6.41252800	-1.25584100	-0.95748800
H	5.60906500	-0.98941600	-2.50315800
H	6.33798800	0.37138400	-1.64844100

**ENTRY: K**  
**MOLECULE: 20**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-1375.623155

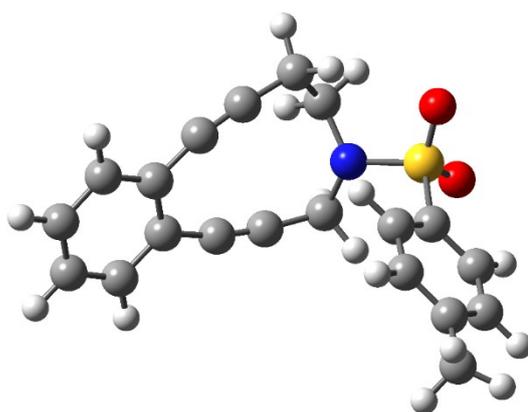


Cartesian coordinates of optimized enediyne **20** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	-3.64844400	0.07824300	-0.54001500
C	-3.33565300	0.54416300	0.77650600
C	-2.74780200	-0.85394900	-1.13937100
C	-2.12754200	0.06358400	1.36694100
C	-1.85194700	-1.63311700	-1.39853000
C	-1.06568400	-0.45919100	1.63721900
C	-0.73951600	-2.57587100	-1.50273600
C	-0.06433000	-2.82673900	-0.13212200
C	0.22559200	-1.14094400	1.74222300
C	-4.81536600	0.54047300	-1.16727900
C	-5.66291100	1.43864600	-0.51811100
C	-5.35817200	1.88917000	0.77065100
C	-4.20195900	1.44542900	1.41289800
N	0.64318200	-1.64260800	0.40915000
C	2.61286100	0.17132600	-0.05233300
C	3.69286000	0.73615900	0.62683600
C	3.97944300	2.08969700	0.43743300
C	3.20232000	2.88433500	-0.41669600
C	2.12217900	2.28558400	-1.08778900
C	1.82295200	0.93661100	-0.91531600
C	3.49759000	4.35429000	-0.59530400
S	2.31393500	-1.59114200	0.11921600
O	3.08111500	-2.05190100	1.28884400
O	2.49895400	-2.26087700	-1.17656800
H	-1.09735900	-3.54247800	-1.88250200
H	0.01798200	-2.22497700	-2.21224200
H	0.62744600	-3.66760700	-0.23841600

H	-0.82381400	-3.10903400	0.60197100
H	0.99046500	-0.44564700	2.10259300
H	0.18501900	-1.96143800	2.47301000
H	-5.05009900	0.18633900	-2.16589600
H	-6.56259200	1.78567000	-1.01737000
H	-6.02000000	2.58675400	1.27493100
H	-3.95924000	1.79385100	2.41167400
H	4.29305000	0.12251100	1.28971200
H	4.82118100	2.53176000	0.96361900
H	1.50654700	2.88400800	-1.75409900
H	0.98102400	0.48708400	-1.43049100
H	4.52399100	4.59445400	-0.30439900
H	3.35502900	4.66583400	-1.63488800
H	2.82677400	4.96426700	0.02244500

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-1375.844952

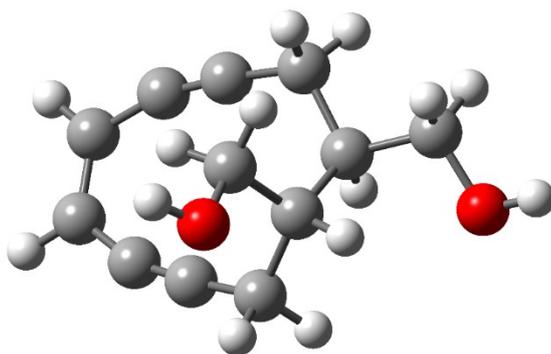


Cartesian coordinates of optimized enediyne **20** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	-3.62287100	0.06769700	-0.53576200
C	-3.31222000	0.53880500	0.77589800
C	-2.72461200	-0.86741000	-1.12625300
C	-2.10862100	0.05940300	1.36858900
C	-1.83887400	-1.64723100	-1.38403400
C	-1.05331800	-0.45833200	1.64171100
C	-0.73414000	-2.59331500	-1.48297300
C	-0.05909200	-2.83513500	-0.11247400
C	0.23533000	-1.13634600	1.74916100
C	-4.78530000	0.52798800	-1.16578200
C	-5.62998900	1.42905600	-0.52441600
C	-5.32739000	1.88463600	0.75914900
C	-4.17629400	1.44281600	1.40439000
N	0.65086200	-1.65042100	0.42147900
C	2.59693300	0.18047900	-0.06041700

C	3.67337000	0.75006000	0.61294700
C	3.94619700	2.10366200	0.42799400
C	3.15810000	2.89268300	-0.41539000
C	2.08107900	2.28914600	-1.08019000
C	1.79566400	0.94016800	-0.91200400
C	3.43913100	4.36408500	-0.58995600
S	2.31299500	-1.58558700	0.10934800
O	3.09821400	-2.04069600	1.26061500
O	2.48395200	-2.25033800	-1.18348400
H	-1.09761400	-3.55939400	-1.85340300
H	0.02215500	-2.25329000	-2.19594500
H	0.62858400	-3.67797400	-0.20972100
H	-0.81783400	-3.10969700	0.62237600
H	0.99835900	-0.43653500	2.09993400
H	0.19778600	-1.94737000	2.48755200
H	-5.01896500	0.16988300	-2.16114600
H	-6.52656400	1.77484500	-1.02589900
H	-5.98782400	2.58484900	1.25740100
H	-3.93576200	1.79523700	2.40019500
H	4.28164200	0.13968100	1.26836700
H	4.78627700	2.54997500	0.94927200
H	1.45687200	2.88411000	-1.73849300
H	0.95519700	0.48635200	-1.42187900
H	4.46376600	4.61124500	-0.30605900
H	3.28582300	4.67759500	-1.62540100
H	2.76830900	4.96361200	0.03476100

**ENTRY: L**  
**MOLECULE: 21**



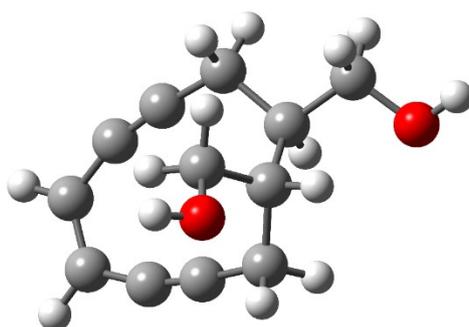
<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-616.032216

Cartesian coordinates of optimized enediyne **21** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	3.49296600	-0.91367700	0.18808400
C	3.53162400	0.17832500	-0.62961800

C	2.23110400	-1.40245300	0.62137900
C	2.31505400	0.80167800	-1.01347800
C	1.03756100	-1.56236400	0.79794500
C	1.14111700	1.09430300	-1.15271200
C	-0.41331100	-1.67982600	0.90819900
C	-1.21069800	-0.85686600	-0.15571400
C	-0.29218000	1.36965200	-1.21656200
C	-1.13668000	0.70805300	-0.08355700
C	-2.67581600	-1.31284300	-0.09244900
C	-0.76295100	1.25144000	1.29641600
O	-3.35967700	-0.78550000	-1.23067500
O	-1.01609400	2.66160500	1.29128900
H	4.41210900	-1.40240600	0.49733000
H	4.48456800	0.56624300	-0.97839500
H	-0.69247400	-2.73517600	0.78553400
H	-0.73482700	-1.40879200	1.92284100
H	-0.83430500	-1.16560300	-1.13810800
H	-0.46193700	2.45124600	-1.16720100
H	-0.69231400	1.03306800	-2.18176100
H	-2.15388200	1.06546800	-0.28106100
H	-2.72414400	-2.41134900	-0.09736800
H	-3.14260500	-0.95596100	0.83972900
H	-1.38133600	0.76787200	2.06741500
H	0.29149900	1.04877000	1.52125500
H	-4.30316900	-0.97284300	-1.15308900
H	-0.60776900	3.05809600	2.07037100

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-616.167174



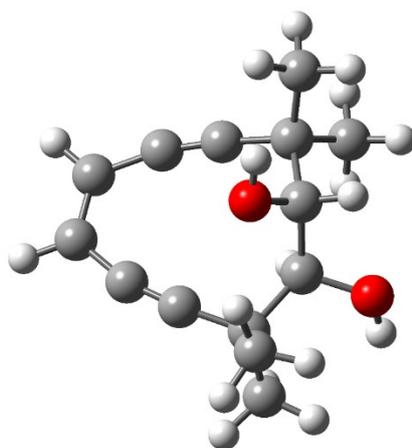
Cartesian coordinates of optimized enediyne **21** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	3.47533500	-0.91254300	0.18179500
C	3.51158900	0.17175300	-0.63800900
C	2.21717400	-1.39664600	0.61888000
C	2.29634800	0.79161900	-1.01816200
C	1.03443700	-1.56552100	0.80670700

C	1.13336400	1.09438500	-1.16068500
C	-0.41325600	-1.67816900	0.91536900
C	-1.20441600	-0.85549000	-0.15104300
C	-0.29621200	1.37069400	-1.21526900
C	-1.13103300	0.70825200	-0.07755000
C	-2.66771700	-1.31086500	-0.09647500
C	-0.74574200	1.24989000	1.29768400
O	-3.34844700	-0.77763000	-1.23313600
O	-0.99906500	2.65990200	1.29709700
H	4.39305500	-1.40034600	0.49021400
H	4.46124800	0.55788600	-0.99191500
H	-0.69484400	-2.73105900	0.79382500
H	-0.73433500	-1.40499500	1.92745900
H	-0.82243500	-1.16263500	-1.12938200
H	-0.46411900	2.45052200	-1.16368800
H	-0.70217800	1.03664200	-2.17673400
H	-2.14838800	1.06414900	-0.26461400
H	-2.71516500	-2.40736900	-0.10817400
H	-3.13744300	-0.96034800	0.83439400
H	-1.35575900	0.76668300	2.07261700
H	0.30894000	1.04852300	1.51278700
H	-4.28748100	-0.97016700	-1.15728200
H	-0.58021900	3.05018000	2.06935400

**ENTRY: M**

**MOLECULE: 22**



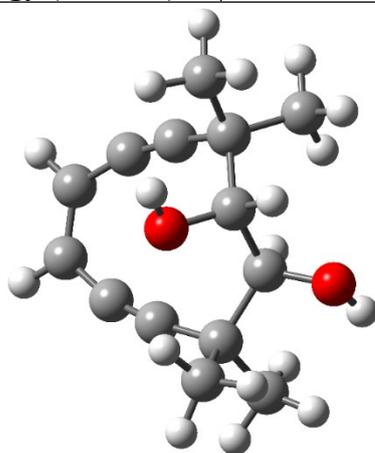
<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-694.665975

Cartesian coordinates of optimized enediyne **22** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	1.43206800	3.09675500	-0.29832400
C	0.12453500	3.40423300	-0.06086600
C	1.83276400	1.73474800	-0.35241500

C	-0.82879600	2.36228200	0.08666900
C	1.90278000	0.52012000	-0.31505800
C	-1.41526700	1.29828100	0.16296800
C	1.81588000	-0.93381500	-0.11614200
C	0.40524900	-1.26925700	0.51769600
C	-1.98008300	-0.05404700	0.04869700
C	-0.80215800	-0.99564200	-0.43167500
O	0.22172200	-0.59994100	1.75853200
O	-1.28599700	-2.30609400	-0.76367400
C	-3.03988800	-0.01582000	-1.09092300
C	-2.68060100	-0.53376300	1.34030000
C	2.00763100	-1.70548700	-1.44428500
C	2.92741500	-1.38960200	0.86539100
H	2.16320000	3.88877200	-0.43356400
H	-0.18721500	4.44360300	-0.00441800
H	0.39947400	-2.35599300	0.68064400
H	-0.42084200	-0.51639100	-1.34112600
H	0.89071900	-0.90675500	2.38199300
H	-1.85423300	-2.24644400	-1.54211300
H	-2.58567200	0.23780900	-2.05523900
H	-3.55961400	-0.97701800	-1.17404200
H	-3.79271500	0.74486400	-0.86804600
H	-2.96933500	-1.58369400	1.22735600
H	-3.58647000	0.05748800	1.50914500
H	-2.02718600	-0.43889300	2.20507500
H	1.88764900	-2.78122500	-1.27749800
H	3.01230200	-1.52445700	-1.83722300
H	1.29124600	-1.39723000	-2.20882400
H	2.90310200	-0.82748200	1.80388600
H	2.82835100	-2.45990800	1.08278300
H	3.91227000	-1.22269900	0.42014900

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-694.813768



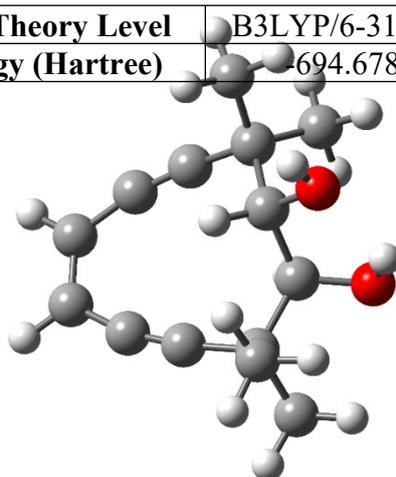
Cartesian coordinates of optimized enediyne **22** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	1.41751900	3.08951900	-0.30019700
C	0.11428700	3.39262700	-0.06112700
C	1.81985300	1.73180600	-0.35470900
C	-0.83295500	2.35032700	0.08793500
C	1.89789900	0.52506700	-0.31795000
C	-1.41595500	1.29287700	0.16398900
C	1.81733500	-0.92524200	-0.11681100
C	0.40960900	-1.26530400	0.51799200
C	-1.97651700	-0.05703000	0.04920300
C	-0.79876900	-0.99750800	-0.42991700
O	0.22451000	-0.59778500	1.75830000
O	-1.28233800	-2.30745400	-0.76137000
C	-3.03336800	-0.02108000	-1.09115600
C	-2.67585800	-0.53801600	1.33926500
C	2.01102400	-1.69707600	-1.44256200
C	2.92917800	-1.37325800	0.86549700
H	2.14572600	3.88151000	-0.43643500
H	-0.20010800	4.42921900	-0.00394600
H	0.40775800	-2.34994800	0.68123800
H	-0.41926400	-0.51937900	-1.33808200
H	0.90979500	-0.88306500	2.36918500
H	-1.85031300	-2.24416200	-1.53549300
H	-2.57878400	0.23764300	-2.05176600
H	-3.54653100	-0.98336300	-1.17874300
H	-3.78916600	0.73370000	-0.86754600
H	-2.96122000	-1.58716800	1.22796000
H	-3.58221100	0.04949100	1.50708900
H	-2.02445000	-0.44006100	2.20263500
H	1.89944900	-2.77178800	-1.27500100
H	3.01177000	-1.50970200	-1.83755500
H	1.29179700	-1.39447700	-2.20412400
H	2.89978700	-0.81091300	1.80175900
H	2.83706500	-2.44198200	1.08415900
H	3.91184000	-1.19989000	0.42251200

**ENTRY: N**

**MOLECULE: 23**

DFT Theory Level	B3LYP/6-31G+(d,p)
Energy (Hartree)	-694.678057

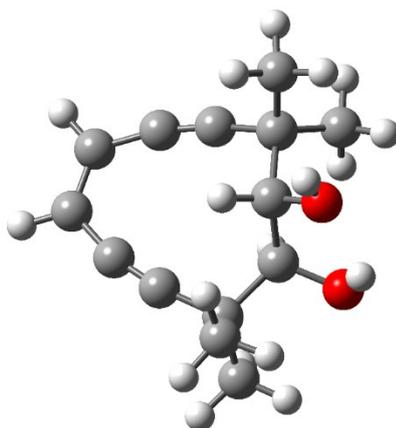


Cartesian coordinates of optimized enediyne **23** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	0.66127300	3.45789700	-0.12421300
C	-0.67319000	3.45024900	0.15911000
C	1.35861800	2.22702500	-0.25355600
C	-1.36462900	2.21467200	0.27110600
C	1.71656700	1.06326000	-0.28295900
C	-1.71956300	1.04914000	0.27742500
C	1.94799200	-0.37920900	-0.09902300
C	0.59638200	-0.94062000	0.48943100
C	-1.95392800	-0.38917500	0.07082600
C	-0.60048700	-0.96656400	-0.51591000
O	-0.78959800	-2.26914200	-1.04159100
O	0.76204700	-2.28841000	0.96171100
C	-2.38282400	-1.10129600	1.37255100
C	-3.06286000	-0.56802800	-0.99627300
C	2.35075300	-1.08550200	-1.41266200
C	3.07596000	-0.56939800	0.94707000
H	1.19034600	4.40038600	-0.23291300
H	-1.20836100	4.38820900	0.27864800
H	0.33626300	-0.29306000	1.33291000
H	-0.35633100	-0.32163100	-1.36501400
H	-0.46999900	-2.89839900	-0.37538300
H	1.07117800	-2.28073900	1.87458600
H	-2.48484300	-2.17570300	1.19110900
H	-3.35009700	-0.71758800	1.71060300
H	-1.66500300	-0.95039600	2.18390300
H	-2.78058800	-0.08669300	-1.93753900
H	-3.22566300	-1.63113600	-1.18765900
H	-3.99613600	-0.11647700	-0.64700900
H	2.44749100	-2.16097900	-1.23847100
H	3.31245100	-0.69998800	-1.76450000
H	1.61373700	-0.93139700	-2.20369100
H	2.80174400	-0.12828200	1.91197400
H	3.29319900	-1.63302400	1.08484700
H	3.99061600	-0.07737900	0.60509800

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
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Energy (Hartree)	-694.825619
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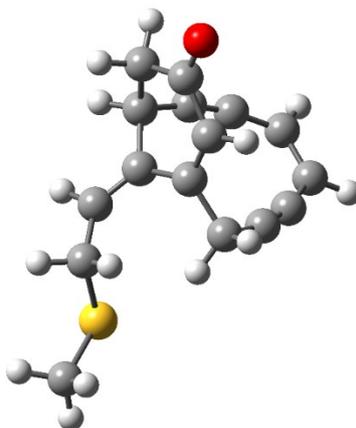
Cartesian coordinates of optimized enediyne **23** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	0.64323900	3.44996100	-0.12414300
C	-0.68613600	3.43660700	0.15973700
C	1.34341300	2.22474900	-0.25402100
C	-1.36974600	2.20065200	0.27186900
C	1.70585300	1.07012100	-0.28271300
C	-1.71821900	1.04090200	0.27664000
C	1.94680200	-0.36661600	-0.09967600
C	0.60089600	-0.93902300	0.48868500
C	-1.94946600	-0.39370200	0.07148100
C	-0.59606700	-0.96977100	-0.51456700
O	-0.78354400	-2.27285800	-1.03668800
O	0.77643100	-2.28576000	0.95856200
C	-2.37604800	-1.10619700	1.37190500
C	-3.05599100	-0.57466300	-0.99581100
C	2.35162200	-1.06992900	-1.41238900
C	3.07505800	-0.54909400	0.94535600
H	1.16810300	4.39262900	-0.23315500
H	-1.22512600	4.37012700	0.27994800
H	0.33798200	-0.29603300	1.33199500
H	-0.35412400	-0.32616500	-1.36255200
H	-0.45326700	-2.89566300	-0.37445800
H	1.08976600	-2.27434900	1.86634700
H	-2.47790100	-2.17886800	1.19106900
H	-3.34141600	-0.72365400	1.71109900
H	-1.65803400	-0.95501500	2.18060700
H	-2.77547600	-0.08920900	-1.93338300
H	-3.21363700	-1.63594500	-1.19084800
H	-3.98998000	-0.12916200	-0.64630400
H	2.45729800	-2.14283800	-1.23862700
H	3.30756200	-0.67775800	-1.76710000
H	1.61190000	-0.92201200	-2.19967900

H	2.79815900	-0.10966500	1.90815600
H	3.29892400	-1.60924900	1.08427800
H	3.98491400	-0.05220700	0.60349500

**ENTRY: O**  
**MOLECULE: 24**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-1091.407949

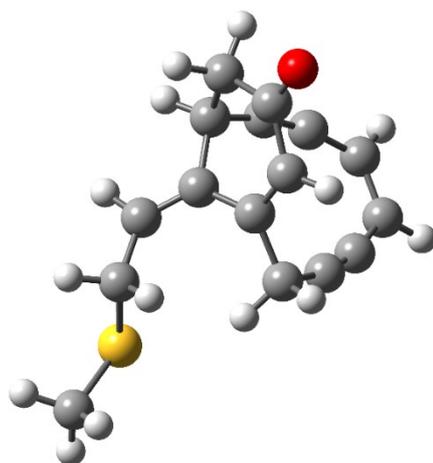


Cartesian coordinates of optimized enediyne **24** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	-2.50930700	2.90352800	-0.83090900
C	-1.86793300	3.40150400	0.26381700
C	-2.25323200	1.56868200	-1.24740300
C	-0.96807000	2.57094100	0.98429400
C	-0.27557200	1.68103100	1.44153800
C	-1.86370200	0.42862600	-1.41936600
C	0.38963800	0.41235100	1.76577800
C	-0.30194700	-0.64916100	0.90193000
C	-1.37534600	-1.31705300	1.38591000
C	-2.26739800	-2.12347800	0.53340000
O	-3.16817900	-2.80428200	1.01012200
C	-2.05727000	-2.06127300	-0.97900200
C	-1.17825500	-0.87266500	-1.44990100
C	0.05070000	-0.79492100	-0.53371800
C	1.29047900	-0.93577400	-1.03821400
H	-0.84512300	-1.07817500	-2.47418100
H	1.38908700	-1.00704200	-2.12023100
C	2.57573400	-1.06281000	-0.27742600
S	3.57332500	0.49059500	-0.40296900
C	5.16833500	-0.12015800	0.24873000
H	-3.20393900	3.52552300	-1.38817300
H	-2.04739800	4.42320100	0.58608400
H	0.27336900	0.16666100	2.82781500

H	1.46089200	0.49432300	1.55595500
H	-1.67698500	-1.22516400	2.42618900
H	-3.04113000	-2.05064900	-1.45594200
H	-1.56174300	-2.99623300	-1.27266300
H	2.40830400	-1.31080700	0.77447000
H	3.17213300	-1.86836000	-0.72063600
H	5.86008600	0.72518500	0.22844800
H	5.57206400	-0.92050900	-0.37796100
H	5.07148500	-0.46944100	1.28060100

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-1091.573622



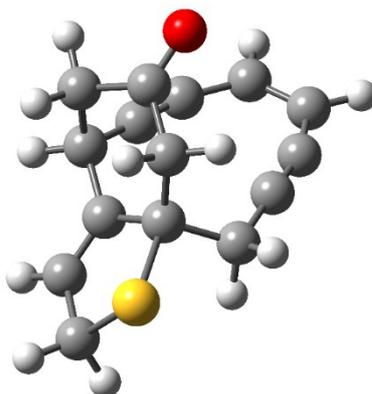
Cartesian coordinates of optimized enediyne **24** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	-2.51389900	2.89035700	-0.82508800
C	-1.87441100	3.39063100	0.26378500
C	-2.25419800	1.55985300	-1.24120700
C	-0.97127900	2.56757000	0.98206900
C	-0.28069400	1.68323400	1.43300500
C	-1.86261700	0.42844100	-1.41308000
C	0.38809700	0.42120100	1.75743300
C	-0.30003100	-0.64481500	0.89875500
C	-1.36584500	-1.31431400	1.38343200
C	-2.25453000	-2.12806100	0.53548600
O	-3.14087800	-2.81505800	1.01156700
C	-2.05192300	-2.05753000	-0.97714100
C	-1.17712600	-0.86818100	-1.44827300
C	0.05205900	-0.79125000	-0.53522100
C	1.28752200	-0.93389400	-1.03667700
H	-0.84581800	-1.06918100	-2.47177600
H	1.38822200	-1.00932000	-2.11644000
C	2.56833000	-1.05898500	-0.27304800

S	3.56679700	0.49179300	-0.40871800
C	5.15812400	-0.11343800	0.25394300
H	-3.21148200	3.50758600	-1.38032000
H	-2.05728300	4.41009800	0.58481900
H	0.27591300	0.17879700	2.81862800
H	1.45658800	0.50649200	1.54423900
H	-1.66634200	-1.22247400	2.42231500
H	-3.03691200	-2.04549000	-1.44729700
H	-1.55997800	-2.99053400	-1.27586800
H	2.40056600	-1.29606100	0.77884000
H	3.16554300	-1.86461100	-0.70928100
H	5.84725400	0.73135500	0.23019000
H	5.56193400	-0.91598800	-0.36592200
H	5.05457600	-0.45380500	1.28578200

**ENTRY: P**  
**MOLECULE: 25**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-1052.099296

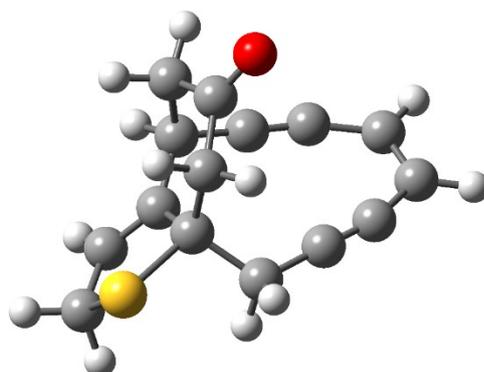


Cartesian coordinates of optimized enediyne **25** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	-3.77223500	-0.72899000	0.68752400
C	-3.56120500	-1.50745600	-0.41347400
C	-2.65968700	-0.05268000	1.25354100
C	-2.23970100	-1.62951500	-0.91681400
C	-1.03146800	-1.54577600	-1.04086100
C	-1.53203900	0.36573000	1.43874900
C	0.42580500	-1.49725800	-1.08588000
C	1.12657900	-0.19849500	-0.53365900
C	0.76690700	1.04121200	-1.39834400
C	-0.24783600	2.01975000	-0.80968200
O	-1.02128100	2.62792200	-1.52516200
C	-0.15940200	2.27657200	0.68646500
C	-0.18740400	0.94533100	1.49806000

C	0.93598000	0.04909900	0.97035000
C	1.90726400	-0.41723800	1.76348700
C	3.10225500	-1.04714400	1.10613200
S	2.96778700	-0.56380100	-0.66643300
H	0.05416200	1.18132800	2.54137600
H	-4.76772400	-0.61551200	1.10494400
H	-4.38749100	-2.02708200	-0.88894700
H	0.77548000	-1.62493700	-2.11729200
H	0.82030800	-2.35327600	-0.52529100
H	1.67558700	1.64234600	-1.53885600
H	0.41578900	0.75209000	-2.39206600
H	-0.97614400	2.93757600	0.98271100
H	0.79643300	2.78014800	0.88711300
H	1.87329600	-0.32638000	2.84688500
H	3.12328100	-2.13795800	1.22347500
H	4.03979400	-0.64974900	1.50661800

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-1052.257496



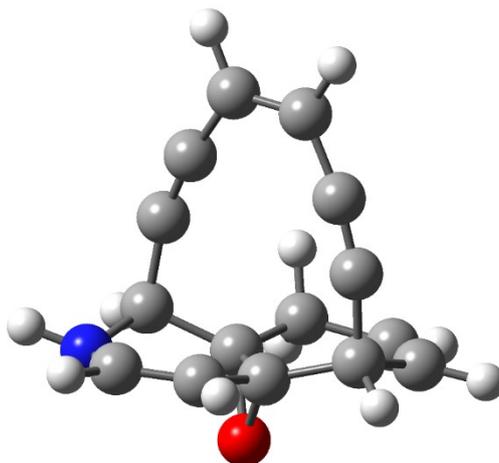
Cartesian coordinates of optimized enediyne **25** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	-3.75746800	-0.72541100	0.68487900
C	-3.54567000	-1.50995800	-0.40551700
C	-2.64644200	-0.04979100	1.24533700
C	-2.22586800	-1.63456200	-0.90197700
C	-1.02619400	-1.55807800	-1.03789400
C	-1.53160700	0.37777900	1.43644800
C	0.42745700	-1.50380000	-1.07969700
C	1.11964000	-0.20044100	-0.53305500
C	0.75648300	1.03264000	-1.40169300
C	-0.25326300	2.01719500	-0.81530300
O	-1.02693600	2.61711600	-1.52484700
C	-0.15441100	2.27810100	0.67867200
C	-0.18831900	0.95112700	1.49362600
C	0.93051000	0.04972100	0.96927700
C	1.89761600	-0.41437600	1.76081600
C	3.09164300	-1.04421200	1.10661600
S	2.96314800	-0.55498800	-0.66327300

H	0.05324500	1.18808200	2.53450200
H	-4.75147000	-0.60695000	1.09968300
H	-4.36905500	-2.03185500	-0.87935600
H	0.77901200	-1.63566500	-2.10797100
H	0.82301800	-2.35384300	-0.51449600
H	1.66332400	1.63087300	-1.55107500
H	0.40014600	0.73862500	-2.38990900
H	-0.96362900	2.94448100	0.97643200
H	0.80417300	2.77525800	0.87120500
H	1.86444400	-0.31928400	2.84189100
H	3.11033700	-2.13336000	1.21855600
H	4.02692100	-0.64910100	1.50846900

**ENTRY: Q**  
**MOLECULE: 26**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-708.002558

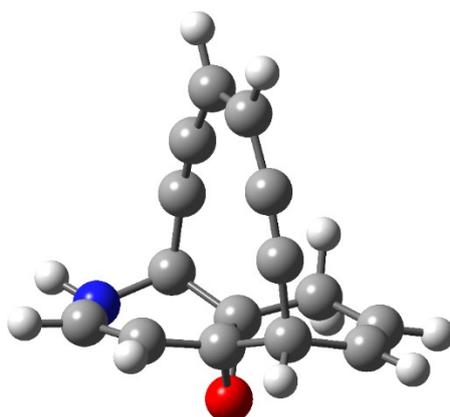


Cartesian coordinates of optimized enediyne **26** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

N	-0.61416200	2.66336600	-0.01373200
C	-0.42262000	2.29161500	1.31195300
C	-0.58284400	1.02528100	1.73906500
C	-1.05256700	-0.00720300	0.78435100
C	-1.11626700	0.31937200	-0.64876000
C	-0.41647100	1.63962100	-1.05188100
C	-0.76896700	-1.47764900	1.14986600
C	-1.33446900	-2.45035200	0.12828600
C	-1.47952700	-2.12182500	-1.15886900
C	-1.13028300	-0.76782600	-1.71387800
O	-2.31728000	0.35061400	0.12816700
C	1.01489700	1.26522400	-1.18161800
C	2.10891200	0.78037400	-0.94684300

C	3.25802400	0.05121400	-0.54503300
C	3.14463600	-0.99967300	0.32123500
C	1.87787500	-1.39472000	0.81962300
C	0.70782900	-1.55476900	1.12155900
H	-0.22146800	3.56156800	-0.26332900
H	-0.16506200	3.09997500	1.98906300
H	-0.45100800	0.77056100	2.78404600
H	-0.82472900	2.03233000	-1.98989600
H	-1.16162200	-1.70433700	2.14940200
H	-1.58280900	-3.44753600	0.48044600
H	-1.86480900	-2.85927200	-1.85928300
H	-1.86176300	-0.47931900	-2.48205600
H	-0.15297700	-0.80840400	-2.21404200
H	4.23676000	0.33239900	-0.92391700
H	4.03791400	-1.53854300	0.62602400

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-708.145531



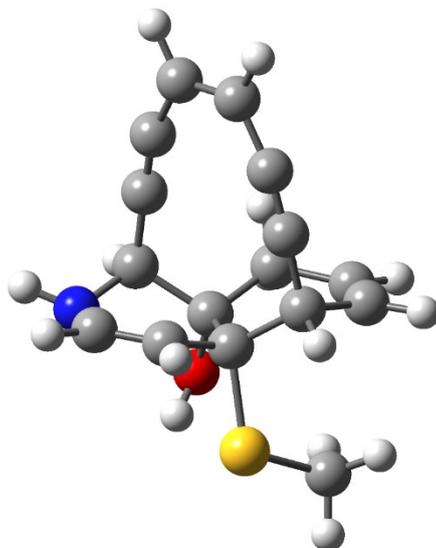
Cartesian coordinates of optimized enediyne **26** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

N	-0.62526400	2.65801100	-0.02324600
C	-0.44224900	2.29150000	1.30316700
C	-0.59795900	1.03009300	1.73254900
C	-1.05575700	-0.00804600	0.78056800
C	-1.11438800	0.31186300	-0.65172600
C	-0.41455600	1.63067200	-1.05487500
C	-0.76054000	-1.47405000	1.14946100
C	-1.32268700	-2.45166100	0.13246100
C	-1.46338700	-2.13021900	-1.15166200
C	-1.11403200	-0.77968000	-1.70982800
O	-2.31671100	0.33920600	0.11712600
C	1.01419800	1.26022300	-1.16811900
C	2.10723400	0.78915200	-0.94063100
C	3.25300000	0.06198900	-0.53636700

C	3.13985200	-0.98469800	0.32739700
C	1.87668900	-1.38303300	0.82299400
C	0.71233900	-1.54180000	1.11724300
H	-0.23730400	3.55642600	-0.27231900
H	-0.19548500	3.10212900	1.97875900
H	-0.47365500	0.78154100	2.77791000
H	-0.81429400	2.01595100	-1.99729600
H	-1.14818700	-1.69986800	2.14880300
H	-1.57129400	-3.44541900	0.48826500
H	-1.84580300	-2.86932800	-1.84901500
H	-1.83811900	-0.49823600	-2.48493400
H	-0.13410100	-0.81919200	-2.20075400
H	4.23039800	0.34382500	-0.91279400
H	4.03183800	-1.52139600	0.63329500

**ENTRY: R**  
**MOLECULE: 27**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-1146.737304

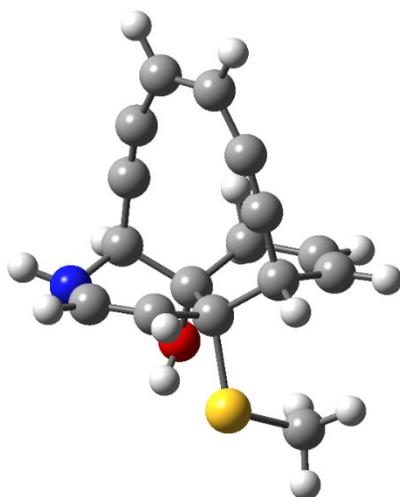


Cartesian coordinates of optimized enediyne **27** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

N	-0.34675400	2.67856900	-0.00212800
C	-0.25586900	2.20579400	-1.30673400
C	0.19639300	0.97418600	-1.59670000
C	0.79893700	0.05404300	-0.56341300
C	0.54595400	0.55847000	0.94194100
C	-0.60877800	1.64139900	1.00776000
C	0.35086200	-1.44093100	-0.81113800
C	0.80761300	-2.35505500	0.31281000

C	0.76281200	-1.93450500	1.57928200
C	0.22182300	-0.58167700	1.94280200
O	1.69676300	1.20301400	1.47646200
C	-1.96107100	1.08449800	0.85312300
C	-3.04248500	0.59520000	0.57807200
C	-4.06029000	-0.24664000	0.05944100
C	-3.69959700	-1.31992900	-0.70535100
C	-2.32541900	-1.58097900	-0.93473700
C	-1.10789900	-1.54583300	-0.94808700
H	-0.92613700	3.50047700	0.10853300
H	-0.57399000	2.88891000	-2.08869700
H	0.24320600	0.65555800	-2.63204300
H	-0.49481500	2.10135600	1.99450200
H	0.81975000	-1.74692300	-1.75350000
H	1.14342200	-3.35547100	0.05367700
H	1.07403600	-2.59325300	2.38686500
H	0.60699600	-0.25712300	2.91418700
H	-0.86772300	-0.67019500	2.04614900
H	-5.10763600	-0.04154000	0.25953900
H	-4.46093400	-1.97019500	-1.12694000
H	2.19483200	1.60626800	0.74422900
S	2.62061600	0.23002800	-1.06962300
C	3.64900400	-0.91074400	-0.06593300
H	3.45974400	-1.95692200	-0.30930700
H	4.67871700	-0.66087700	-0.33946300
H	3.50192300	-0.73840500	1.00061100

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-1146.916458



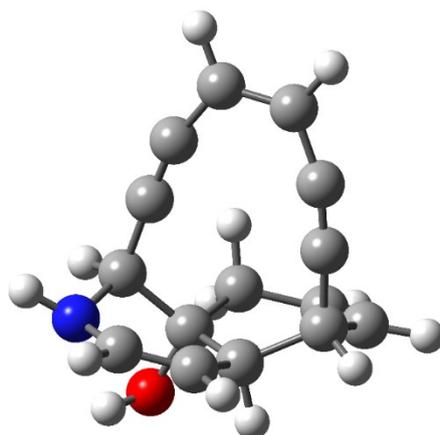
Cartesian coordinates of optimized enediyne **27** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

N	-0.35029600	2.67710700	-0.00390700
C	-0.25782700	2.20164200	-1.30556600
C	0.19428500	0.97439500	-1.59359700
C	0.79538800	0.05594600	-0.56087000
C	0.53983100	0.55890700	0.94347800
C	-0.61363800	1.64176400	1.00675100
C	0.35391000	-1.43927100	-0.80960300
C	0.80701800	-2.35043600	0.31632200
C	0.75503600	-1.93163400	1.57765600
C	0.20991900	-0.58193700	1.93894800
O	1.68839100	1.20249000	1.48151600
C	-1.96212500	1.08652900	0.85070100
C	-3.02961500	0.58718200	0.57313600
C	-4.04404600	-0.25253600	0.05472700
C	-3.68196500	-1.32092000	-0.70753100
C	-2.31024800	-1.57643300	-0.93427800
C	-1.10008700	-1.54968600	-0.95377200
H	-0.93041900	3.49683300	0.10330800
H	-0.57435400	2.88223000	-2.08785900
H	0.24322200	0.65598500	-2.62680700
H	-0.50163900	2.10102100	1.99178100
H	0.82764400	-1.74372300	-1.74758900
H	1.14550800	-3.34834500	0.05954700
H	1.06306700	-2.58882900	2.38511300
H	0.58636500	-0.25903300	2.91207300
H	-0.87834600	-0.67202700	2.03395500
H	-5.08988300	-0.04868100	0.25412100
H	-4.43927500	-1.97219300	-1.13010300
H	2.19583800	1.58708100	0.74975400
S	2.61837000	0.23622300	-1.06431800
C	3.64211000	-0.91392900	-0.06805600
H	3.44906400	-1.95517200	-0.31954100
H	4.67018300	-0.66487000	-0.34131500
H	3.49638800	-0.74700200	0.99719200

**ENTRY: S**

**MOLECULE: 28**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-709.247931



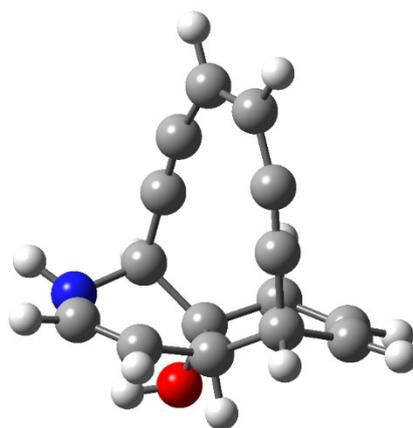
Cartesian coordinates of optimized enediyne **28** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

```

N      1.13582600 -2.38558300  0.08362500
C      0.87422400 -2.05389600  1.42451000
C      0.83368700 -0.78604400  1.86243600
C      1.11160300  0.39597200  0.97155900
C      1.40579300 -0.02662900 -0.50849500
C      0.70496900 -1.37759700 -0.90607800
C      0.10937700  1.58698400  1.17310500
C      0.49692100  2.72560600  0.24215500
C      0.97618600  2.47342900 -0.97967600
C      1.09768000  1.08124600 -1.54125500
O      2.81538000 -0.28573400 -0.61748900
C     -0.75506700 -1.29408300 -1.01869200
C     -1.97126900 -1.22497100 -1.01397500
C     -3.31030900 -0.83932200 -0.74499500
C     -3.53571700  0.20297200  0.10917800
C     -2.42862200  0.87903300  0.68044100
C     -1.29615100  1.22214900  0.96983300
H      0.85864400 -3.32623900 -0.16822100
H      0.74764200 -2.89708300  2.09668000
H      0.66199100 -0.60133600  2.91868600
H      1.13643100 -1.66392000 -1.87222000
H      0.23911600  1.91657600  2.21310600
H      0.36004200  3.74403000  0.59576200
H      1.24378200  3.29887000 -1.63574400
H      1.88374400  1.03918300 -2.30114500
H      0.15317200  0.83961000 -2.04964600
H     -4.14190400 -1.36364700 -1.20592700
H     -4.55191000  0.51103000  0.33836900
H      2.98675500 -1.13629200 -0.18053600
H      2.06883100  0.83508200  1.28505800

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<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-709.393338



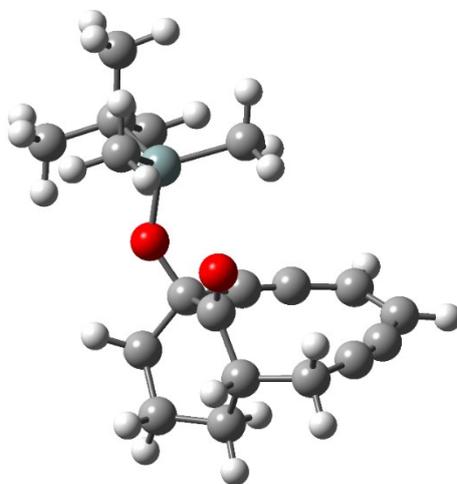
Cartesian coordinates of optimized enediyne **28** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

N	1.14822100	-2.37830300	0.08379100
C	0.88455900	-2.04727400	1.42267300
C	0.83517100	-0.78435900	1.85976300
C	1.10543100	0.39865800	0.97063800
C	1.40059000	-0.01871200	-0.50941000
C	0.71205300	-1.37470800	-0.90684800
C	0.09905100	1.58433900	1.17391400
C	0.47806000	2.72352300	0.24262600
C	0.95176600	2.47523700	-0.97651400
C	1.07743700	1.08567800	-1.53843100
O	2.81182500	-0.26343800	-0.62241500
C	-0.74476300	-1.30239400	-1.02144700
C	-1.95282200	-1.22658500	-1.00942900
C	-3.29142500	-0.85124700	-0.74412900
C	-3.52311300	0.18500200	0.10792800
C	-2.42169000	0.86236700	0.67912400
C	-1.30153100	1.21355900	0.97488600
H	0.87802000	-3.31946800	-0.16627400
H	0.76391500	-2.88956300	2.09415900
H	0.66341000	-0.60172200	2.91436000
H	1.14597700	-1.65671300	-1.87085500
H	0.22899300	1.91464100	2.21151500
H	0.33835800	3.73928500	0.59675200
H	1.21277100	3.30083400	-1.63186500
H	1.85584300	1.04844000	-2.30350600
H	0.13215500	0.83814200	-2.03825700
H	-4.11713800	-1.37979000	-1.20651400
H	-4.53908000	0.48803200	0.33606800
H	2.99270800	-1.10490200	-0.17966500
H	2.05928000	0.83991300	1.28478400

**ENTRY: T**

**MOLECULE: 29**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-1179.609428

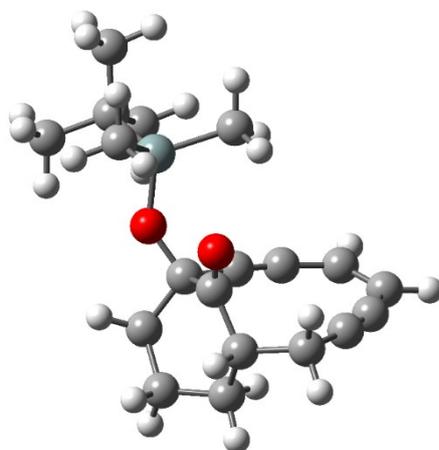


Cartesian coordinates of optimized enediyne **29** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

Si	-2.11920800	-0.09345600	0.69713700
C	-1.46428500	1.41919100	1.61396200
C	-2.63095200	-1.43260800	1.92180100
C	-3.60061400	0.38257800	-0.43360500
C	-4.76137100	0.93330100	0.42506000
C	-3.16913900	1.46353700	-1.44827800
C	-4.09468000	-0.85797900	-1.21033500
O	-1.00057300	-0.75949800	-0.39551000
C	0.38551700	-0.69724500	-0.60629300
C	0.85126800	0.67841300	-0.86929800
C	1.34809600	1.78437500	-0.97794300
C	2.10974700	2.98145400	-0.91118400
C	3.24101000	3.01234300	-0.15056300
C	3.62553600	1.84405900	0.55953900
C	3.69120700	0.72502800	1.03251700
C	3.59434000	-0.66895500	1.45784800
C	2.66878400	-1.51404900	0.52497700
C	3.12761700	-1.58463400	-0.93844200
C	2.08515500	-2.34405000	-1.76976500
C	0.70613600	-1.64505800	-1.81081100
C	1.19063800	-1.12080200	0.67460400
O	0.64322800	-1.15097200	1.75834900
H	-2.24763100	1.81809700	2.26997200
H	-0.60882500	1.15101900	2.24034800
H	-1.15271800	2.21905400	0.93605700
H	-3.45372000	-1.09136300	2.56100300
H	-2.96024600	-2.34136000	1.40632600
H	-1.78393100	-1.69438900	2.56187600

H	-5.61093700	1.20940200	-0.21582700
H	-5.12771700	0.19364200	1.14653500
H	-4.47125900	1.83162800	0.98255800
H	-2.85005100	2.38847900	-0.95408900
H	-2.34342200	1.11941000	-2.08038600
H	-4.00901500	1.72108400	-2.10994000
H	-4.92782700	-0.58420300	-1.87392700
H	-3.30061200	-1.28579300	-1.83148700
H	-4.45813100	-1.64506400	-0.53954700
H	1.79037800	3.86167300	-1.46139100
H	3.83812400	3.91761400	-0.09222300
H	4.58707400	-1.13640400	1.47700500
H	3.19612200	-0.72445700	2.47811100
H	2.69656500	-2.53397200	0.93729500
H	3.28141600	-0.57839400	-1.34059900
H	4.09578200	-2.09755300	-0.98631000
H	2.44912500	-2.48767600	-2.79251600
H	1.97096000	-3.34959100	-1.34292800
H	-0.09506700	-2.38875500	-1.81687700
H	0.59916200	-1.05338900	-2.72441200

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-1179.815125



Cartesian coordinates of optimized enediyne **29** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

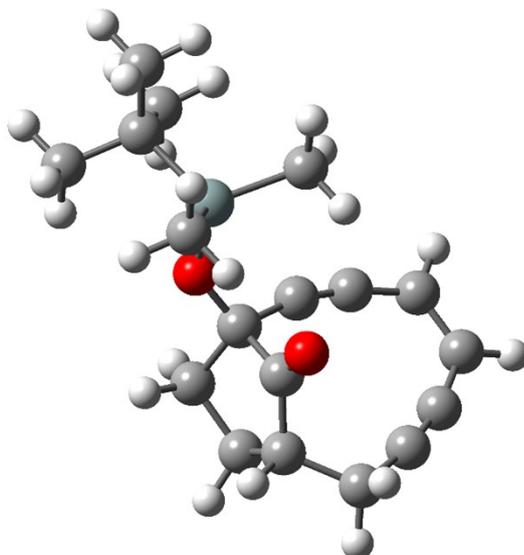
Si	-2.12655500	-0.09519600	0.70022800
C	-1.47687200	1.40612800	1.63012400
C	-2.63623400	-1.44557400	1.90583000
C	-3.59912300	0.38549000	-0.43540400
C	-4.77242400	0.91300900	0.41809500
C	-3.16511400	1.48443800	-1.42729900
C	-4.07334300	-0.84626200	-1.23533900

O	-0.99760100	-0.74322900	-0.38773000
C	0.38698900	-0.68883100	-0.60304600
C	0.85707600	0.68066100	-0.86823100
C	1.35463800	1.77873600	-0.97349800
C	2.11572100	2.97172400	-0.90385700
C	3.24170100	2.99943000	-0.14384600
C	3.62241300	1.83224700	0.56282500
C	3.69255300	0.72061900	1.03314700
C	3.59609000	-0.67118700	1.45269100
C	2.66921300	-1.51075600	0.51910500
C	3.12396100	-1.57209500	-0.94426100
C	2.08321900	-2.32848700	-1.77742400
C	0.70018600	-1.63960000	-1.80485500
C	1.19191100	-1.11889500	0.67659800
O	0.64886900	-1.15668800	1.75406800
H	-2.26496100	1.81403600	2.27169100
H	-0.63746800	1.12815200	2.27075900
H	-1.14406900	2.20124000	0.95979700
H	-3.45730800	-1.11385500	2.54915200
H	-2.96445800	-2.34727700	1.38140900
H	-1.79067700	-1.71366800	2.54224800
H	-5.61429400	1.19380500	-0.22753600
H	-5.14127200	0.15950400	1.12084500
H	-4.49586200	1.80182500	0.99383200
H	-2.86437600	2.40378500	-0.91566200
H	-2.32751500	1.15905100	-2.05044000
H	-3.99684600	1.74105300	-2.09629000
H	-4.89679200	-0.56826500	-1.90601400
H	-3.26833500	-1.25980400	-1.84857500
H	-4.44119700	-1.64317100	-0.58176200
H	1.79886300	3.85169900	-1.45231000
H	3.83911500	3.90210200	-0.08208500
H	4.58743600	-1.13728300	1.46925400
H	3.20072400	-0.72958000	2.47190200
H	2.69652600	-2.53184800	0.92363600
H	3.27491100	-0.56513400	-1.34011900
H	4.09130500	-2.08176600	-0.99780700
H	2.44287700	-2.45941600	-2.80115500
H	1.97721600	-3.33712100	-1.36114400
H	-0.09472500	-2.38686900	-1.79774300
H	0.57744000	-1.05389400	-2.71790400

**ENTRY: U**  
**MOLECULE: 30**

DFT Theory Level	B3LYP/6-31G+(d,p)
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Energy (Hartree)	-1140.296648
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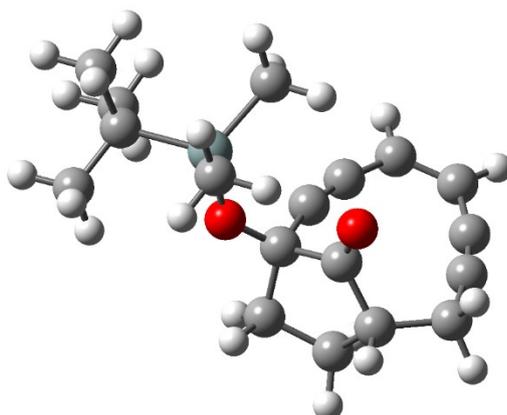


Cartesian coordinates of optimized enediyne **30** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

Si	2.10341800	-0.16117300	-0.62376900
C	1.50715600	1.17420200	-1.81299500
C	2.50903000	-1.73928100	-1.57278700
C	3.61093100	0.43199400	0.40662300
C	4.81310100	0.70555200	-0.52484900
C	3.25289500	1.73060600	1.16194600
C	4.00495400	-0.65162300	1.43448400
O	0.95096100	-0.52522200	0.57467300
C	-0.43962200	-0.42792800	0.67160800
C	-0.98430700	0.93691400	0.56219300
C	-1.68957600	1.91877100	0.41153900
C	-2.69227300	2.88512600	0.13686500
C	-3.91514500	2.46859300	-0.29982600
C	-4.15192700	1.08028300	-0.48606400
C	-4.08412300	-0.13185000	-0.56872100
C	-3.77792600	-1.56202000	-0.58492400
C	-2.46812300	-1.87906300	0.19496500
C	-2.42868500	-1.46512100	1.68199700
C	-0.95351900	-1.11271100	1.96402800
C	-1.22125900	-1.23669500	-0.42778900
O	-0.85218700	-1.37234800	-1.57240900
H	2.29812100	1.40756900	-2.53611800
H	0.63480300	0.82386500	-2.37270300
H	1.23392900	2.10110700	-1.30007100
H	3.32840000	-1.57541200	-2.28254000
H	2.80552200	-2.55021500	-0.89865200
H	1.63186800	-2.06914100	-2.13747500
H	5.67468500	1.05679300	0.06065900

H	5.13246500	-0.19516100	-1.06167200
H	4.59100300	1.47980600	-1.26877600
H	3.01225000	2.55109000	0.47601600
H	2.39522600	1.58731400	1.82792200
H	4.10237500	2.05901700	1.77789900
H	4.85695100	-0.30996100	2.04000700
H	3.17885300	-0.87677000	2.11694500
H	4.30586600	-1.58794000	0.94990200
H	-2.48661400	3.94211200	0.27783300
H	-4.69907600	3.19223000	-0.50329500
H	-4.60295600	-2.14140500	-0.15123000
H	-3.65723400	-1.90722800	-1.61954700
H	-2.30241300	-2.96218900	0.10418200
H	-3.06210300	-0.58734500	1.84214700
H	-2.79097500	-2.25937600	2.34112100
H	-0.34874700	-2.01742100	2.09860600
H	-0.81973300	-0.47885200	2.84372900

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-1140.495397



Cartesian coordinates of optimized enediyne **30** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

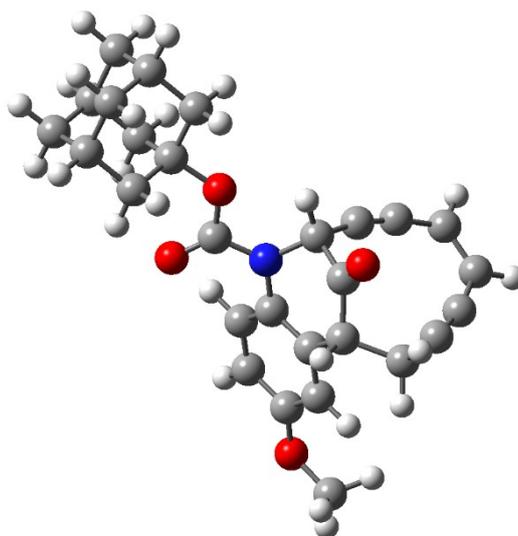
Si	2.10964300	-0.16926800	-0.62536600
C	1.51957500	1.14470000	-1.83452100
C	2.52149300	-1.75786900	-1.54464500
C	3.60537200	0.43857500	0.40926500
C	4.81800200	0.69004900	-0.51238100
C	3.24229300	1.75104500	1.13458800
C	3.98306200	-0.62595200	1.46072800
O	0.94546000	-0.51600100	0.56167300
C	-0.44353800	-0.42184400	0.66546300
C	-0.99011000	0.93738900	0.55440500
C	-1.68593600	1.91662700	0.40160400
C	-2.68589100	2.87998500	0.12463200
C	-3.90595200	2.46381500	-0.30550000
C	-4.14484200	1.07848000	-0.48365800
C	-4.08335100	-0.12674300	-0.56160800

C	-3.78261400	-1.55412800	-0.57388600
C	-2.47202600	-1.87211300	0.20052900
C	-2.42639400	-1.45418100	1.68448800
C	-0.95148500	-1.10316800	1.95997200
C	-1.22602700	-1.23730300	-0.42991300
O	-0.85755400	-1.38292300	-1.56546700
H	2.31615900	1.38194100	-2.54732200
H	0.66180700	0.77846700	-2.40312100
H	1.22685400	2.07091900	-1.33528100
H	3.33757300	-1.60297500	-2.25738100
H	2.82194000	-2.55504700	-0.85901700
H	1.64752600	-2.10112800	-2.10299100
H	5.67183700	1.04971100	0.07575000
H	5.13992400	-0.22087600	-1.02610800
H	4.60769900	1.44841100	-1.27318000
H	3.01600700	2.55817800	0.43118500
H	2.37539500	1.62368300	1.78872900
H	4.08269900	2.08583600	1.75606100
H	4.82675100	-0.27523900	2.06918200
H	3.14886900	-0.83638100	2.13489400
H	4.28689800	-1.56991600	0.99760600
H	-2.47909600	3.93567700	0.25907100
H	-4.68832200	3.18573600	-0.51127400
H	-4.60716500	-2.12755500	-0.13603300
H	-3.66864700	-1.90249200	-1.60627300
H	-2.30776500	-2.95371200	0.11380100
H	-3.05664700	-0.57675100	1.84472900
H	-2.78647400	-2.24460700	2.34584900
H	-0.34786400	-2.00634000	2.09337900
H	-0.81400300	-0.46858100	2.83584800

**ENTRY: V**

**MOLECULE: 31**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-1438.847824

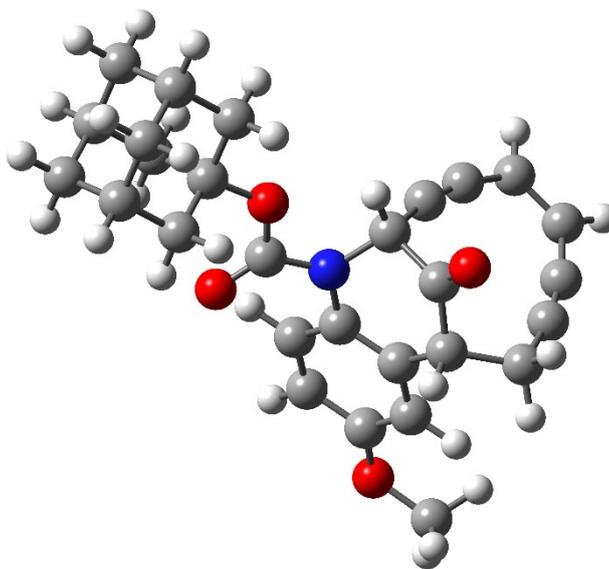


Cartesian coordinates of optimized enediyne **31** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	-3.32395100	-3.00167400	-2.33401800
C	-4.50771800	-2.99167700	-1.65708300
C	-2.16906900	-2.46053800	-1.71025800
C	-4.55749800	-2.44631400	-0.34748700
C	-4.32471100	-1.93486400	0.73150500
C	-3.82418900	-1.30304800	1.94993300
C	-2.48900500	-0.52171500	1.70277700
C	-1.34699900	-1.94100200	-0.97921100
C	-1.55405900	2.00757800	-1.01985900
C	-2.69932100	2.78333000	-1.09165300
C	-3.80288100	2.47852300	-0.28144700
C	-3.73762500	1.39369700	0.59394800
C	-2.57397400	0.61029500	0.68631900
C	-1.47555500	0.92797300	-0.12526700
N	-0.31231100	0.09559300	-0.06797300
C	-0.56357300	-1.34421000	0.10705600
C	-1.36268700	-1.52841300	1.42106800
C	0.96869900	0.63160000	-0.08774100
O	-1.09046500	-2.41326100	2.20501000
O	1.90085800	-0.34538500	-0.03542600
O	1.19874400	1.82777500	-0.14879900
C	5.28010600	0.97534300	1.19231700
C	5.72005800	1.67909600	-0.10982600
C	5.31005000	0.82164500	-1.32694400
C	3.77214700	0.65294300	-1.33790400
C	3.34071100	-0.03812500	-0.03289900
C	3.74213000	0.80586400	1.18874400
C	5.98507500	-0.56215500	-1.23251400
C	4.00276800	-1.42265300	0.05983100
C	5.53850700	-1.26253000	0.06827600
C	5.95610000	-0.40831900	1.28403200

O	-4.89169700	3.29379500	-0.42500900
C	-6.04647700	3.03496500	0.36232600
H	-3.26375800	-3.42171800	-3.33352100
H	-5.40315300	-3.40193900	-2.11523000
H	-4.57107600	-0.63120300	2.38590700
H	-3.61428100	-2.06718400	2.70773700
H	-2.21705300	-0.08923200	2.67740700
H	-0.70247000	2.24257200	-1.64457100
H	-2.76418700	3.62314700	-1.77521400
H	-4.59012100	1.14823300	1.21323600
H	0.39031300	-1.85181400	0.23513200
H	5.56584500	1.58643700	2.05751000
H	6.80781700	1.82867000	-0.10604500
H	5.25897800	2.67294300	-0.17603800
H	5.61760600	1.32280700	-2.25314900
H	3.28111300	1.62529200	-1.42489500
H	3.45989900	0.03870000	-2.19223200
H	3.41069200	0.29823900	2.10390800
H	3.24904300	1.77997100	1.14783200
H	7.07739700	-0.45173500	-1.24418500
H	5.71569100	-1.17455500	-2.10344700
H	3.66194800	-1.92673100	0.97247300
H	3.68271600	-2.03507300	-0.79211700
H	6.00080000	-2.25536300	0.13398600
H	5.66584500	-0.91028600	2.21656200
H	7.04789700	-0.29489700	1.30689900
H	-6.77493100	3.79636700	0.08093700
H	-5.82783100	3.12149100	1.43455200
H	-6.46044400	2.04063300	0.15203800

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-1439.144465



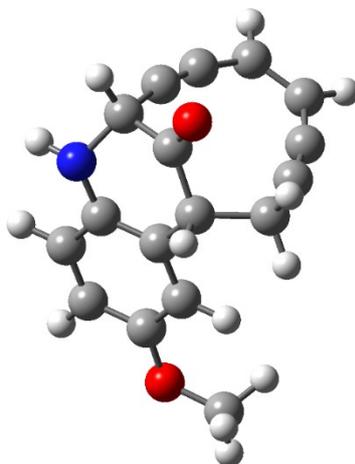
Cartesian coordinates of optimized enediyne **31** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	-3.33774700	-2.97730800	-2.32858000
C	-4.51234000	-2.96795300	-1.64534000
C	-2.17985800	-2.44310300	-1.71244200
C	-4.55199300	-2.43000000	-0.33625400
C	-4.31752200	-1.92760200	0.73814400
C	-3.80833100	-1.30335100	1.95237200
C	-2.47475700	-0.52579800	1.69695900
C	-1.35539100	-1.93255500	-0.99000700
C	-1.55992500	2.00446400	-1.02101200
C	-2.70425300	2.77544700	-1.08700600
C	-3.80174300	2.46913500	-0.27441300
C	-3.72993500	1.38636700	0.59748000
C	-2.56640100	0.60734400	0.68426800
C	-1.47483100	0.92658500	-0.12981500
N	-0.31171500	0.09544600	-0.07962700
C	-0.56312500	-1.34417000	0.08902800
C	-1.35300100	-1.53615800	1.40762500
C	0.96814800	0.63345700	-0.09584100
O	-1.08152000	-2.41966500	2.18158700
O	1.89795300	-0.34260700	-0.03903100
O	1.19677600	1.82212600	-0.15576900
C	5.27460200	0.97526000	1.19299800
C	5.71756100	1.67643400	-0.10736800
C	5.31018800	0.81840600	-1.32270600
C	3.77383400	0.65127900	-1.33733600
C	3.33894400	-0.03680900	-0.03386300
C	3.73820800	0.80713300	1.18651100
C	5.98295000	-0.56422600	-1.22519300
C	3.99878200	-1.42012100	0.06208800
C	5.53298100	-1.26158200	0.07400200
C	5.94838000	-0.40726100	1.28820700
O	-4.89161800	3.28028300	-0.41271800
C	-6.04136100	3.01812600	0.37892800
H	-3.28553900	-3.39232800	-3.32862800
H	-5.41060400	-3.37378800	-2.09755800
H	-4.54964200	-0.63292800	2.39520000
H	-3.59617500	-2.07011200	2.70416600
H	-2.19259300	-0.09394100	2.66679500
H	-0.71388300	2.24099200	-1.64954000
H	-2.77432000	3.61388400	-1.76890800
H	-4.57805700	1.13903900	1.21900400
H	0.38925400	-1.85305500	0.20572900
H	5.55836300	1.58591000	2.05624700
H	6.80329900	1.82552100	-0.10132400
H	5.25803600	2.66852100	-0.17587000
H	5.61974400	1.31699600	-2.24690700
H	3.28526500	1.62235300	-1.42723100

H	3.46395000	0.03730900	-2.19013200
H	3.40543000	0.30152800	2.09989200
H	3.24691800	1.77984100	1.14426600
H	7.07336700	-0.45518000	-1.23470400
H	5.71554300	-1.17629000	-2.09428400
H	3.65560900	-1.92143400	0.97285100
H	3.68071500	-2.03196100	-0.78833000
H	5.99322600	-2.25267800	0.14193600
H	5.65604300	-0.90663200	2.21896700
H	7.03819100	-0.29516700	1.31358000
H	-6.77235900	3.77600200	0.10194600
H	-5.81940800	3.10509000	1.44854400
H	-6.45349100	2.02466400	0.17052700

**ENTRY: W**  
**MOLECULE: 32**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-860.718146

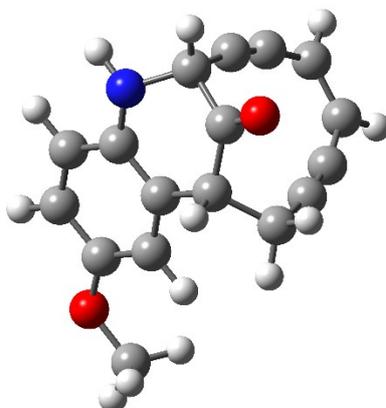


Cartesian coordinates of optimized enediyne **32** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	-3.32395100	-3.00167400	-2.33401800
C	-4.50771800	-2.99167700	-1.65708300
C	-2.16906900	-2.46053800	-1.71025800
C	-4.55749800	-2.44631400	-0.34748700
C	-4.32471100	-1.93486400	0.73150500
C	-3.82418900	-1.30304800	1.94993300
C	-2.48900500	-0.52171500	1.70277700
C	-1.34699900	-1.94100200	-0.97921100
C	-1.55405900	2.00757800	-1.01985900
C	-2.69932100	2.78333000	-1.09165300
C	-3.80288100	2.47852300	-0.28144700
C	-3.73762500	1.39369700	0.59394800

C	-2.57397400	0.61029500	0.68631900
C	-1.47555500	0.92797300	-0.12526700
N	-0.31231100	0.09559300	-0.06797300
C	-0.56357300	-1.34421000	0.10705600
C	-1.36268700	-1.52841300	1.42106800
O	-1.09046500	-2.41326100	2.20501000
O	-4.89169700	3.29379500	-0.42500900
C	-6.04647700	3.03496500	0.36232600
H	-3.26375800	-3.42171800	-3.33352100
H	-5.40315300	-3.40193900	-2.11523000
H	-4.57107600	-0.63120300	2.38590700
H	-3.61428100	-2.06718400	2.70773700
H	-2.21705300	-0.08923200	2.67740700
H	-0.70247000	2.24257200	-1.64457100
H	-2.76418700	3.62314700	-1.77521400
H	-4.59012100	1.14823300	1.21323600
H	0.39031300	-1.85181400	0.23513200
H	-6.77493100	3.79636700	0.08093700
H	-5.82783100	3.12149100	1.43455200
H	-6.46044400	2.04063300	0.15203800
H	0.61251678	0.46867342	-0.14216578

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-860.896923



Cartesian coordinates of optimized enediyne **32** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

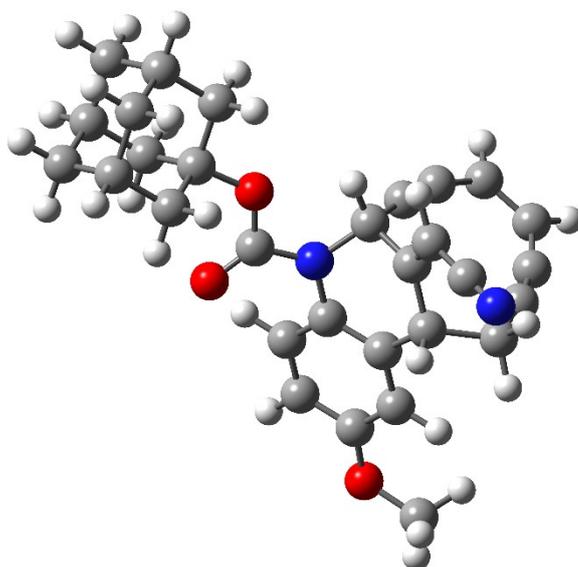
C	-2.62515400	1.79959400	-2.02031600
C	-2.14856500	2.77186700	-1.19874700
C	-2.51334700	0.44637600	-1.61864400
C	-1.56200000	2.41193900	0.03823300
C	-1.12599300	1.84527000	1.01324800
C	-0.67392400	0.97259900	2.08838600
C	-0.41955300	-0.49059000	1.59494300
C	-2.30529000	-0.60407300	-1.05483900
C	1.53783300	-1.77971500	-1.41415100

C	2.70786000	-1.04577900	-1.33756000
C	2.86211600	-0.08392200	-0.33379900
C	1.83555100	0.11383100	0.58617400
C	0.65098500	-0.63440700	0.52315900
C	0.50131800	-1.58898400	-0.48953400
N	-0.66246200	-2.38589500	-0.54265400
C	-1.92191500	-1.72386400	-0.18641900
C	-1.76299100	-1.15287200	1.24426100
O	-2.65431700	-1.23144700	2.05179600
O	4.04570900	0.60563100	-0.34159700
C	4.24914400	1.61120600	0.63834900
H	-3.08748200	2.05561400	-2.96673900
H	-2.22321400	3.81477200	-1.48656100
H	0.23257700	1.36312300	2.55874400
H	-1.43531200	0.92488200	2.87348600
H	-0.08911700	-1.04702200	2.48304400
H	1.41917700	-2.51651100	-2.20247500
H	3.50854500	-1.19230700	-2.05210500
H	1.94846900	0.85224000	1.36754300
H	-2.71157600	-2.47591500	-0.13979600
H	5.23265200	2.03207800	0.43486300
H	4.23958800	1.19308400	1.65171500
H	3.49482900	2.40271700	0.56382500
H	-0.73947300	-2.90983500	-1.40502100

**ENTRY: X**

**MOLECULE: 33**

<b>DFT Theory Level</b>	B3LYP/6-31G+(d,p)
<b>Energy (Hartree)</b>	-1495.164652

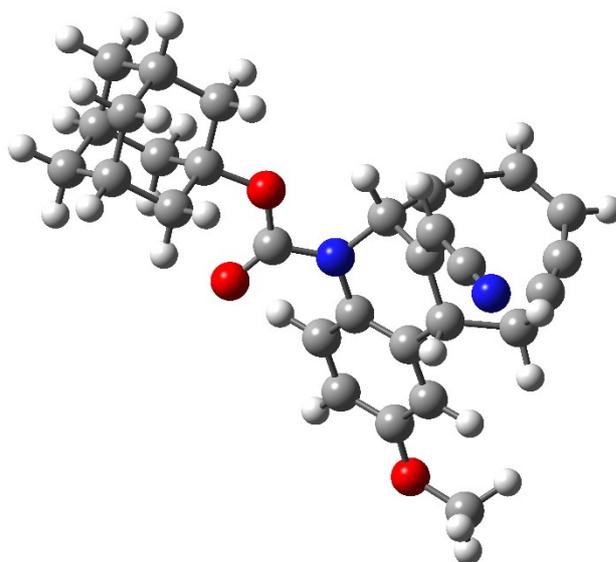


Cartesian coordinates of optimized enediyne **33** at B3LYP/6-31G+(d,p) level of theory, in gas phase.

C	3.10146400	-1.92239300	3.48609800
C	4.32900400	-2.09730300	2.91748700
C	1.99945900	-1.61890100	2.64374900
C	4.46161700	-1.96779800	1.51030500
C	4.25764200	-1.79937500	0.32289200
C	3.86286300	-1.57677500	-1.06299500
C	2.50245000	-0.80054100	-1.22494100
C	1.27307900	-1.37075000	1.70088800
C	1.43486900	2.44090300	0.54526300
C	2.55538000	3.23539800	0.37401900
C	3.67647400	2.72542100	-0.29738000
C	3.65329400	1.41838300	-0.78398300
C	2.51714200	0.60484700	-0.62316300
C	1.39811500	1.13158500	0.03738700
N	0.24973000	0.30207100	0.23742600
C	0.53162200	-1.12845600	0.45729100
C	1.30781900	-1.62279800	-0.76381700
C	-1.03698600	0.78286700	0.03609900
O	-1.95506100	-0.18558200	0.26144100
O	-1.28766200	1.93121800	-0.28739100
C	-5.32294900	0.58552000	-1.38941600
C	-5.80154200	1.67448900	-0.40472200
C	-5.40815800	1.28083800	1.03545600
C	-3.86864200	1.15573400	1.12913800
C	-3.39876600	0.07821400	0.13656600
C	-3.78301300	0.45909900	-1.30303000
C	-6.06319800	-0.06767800	1.39872100
C	-4.04127300	-1.27030300	0.50179900
C	-5.57825900	-1.15317700	0.41457600
C	-5.97783400	-0.76295200	-1.02371500
O	4.73814100	3.57865200	-0.41668700
C	5.91096000	3.12260700	-1.07817500
H	2.96922400	-2.01587000	4.55952300
H	5.19130300	-2.33283500	3.53437800
H	4.64327400	-1.02969500	-1.60290000
H	3.76905500	-2.53741500	-1.58184600
H	2.38907900	-0.68691200	-2.31264300
H	0.56798700	2.83309900	1.06052900
H	2.58733900	4.24925500	0.75833400
H	4.51949900	1.02050300	-1.29588400
H	-0.42674500	-1.64361600	0.49510500
H	-5.59747600	0.86636400	-2.41368600
H	-6.89062400	1.79323100	-0.47688200
H	-5.35391300	2.64186500	-0.66613900
H	-5.74236600	2.05667300	1.73538100
H	-3.39242900	2.11087400	0.89611800
H	-3.56887700	0.86750400	2.14495500

H	-3.42348100	-0.31671100	-1.99137700
H	-3.30374200	1.40140300	-1.57932900
H	-7.15681900	0.01849200	1.35429100
H	-5.80567100	-0.34868600	2.42868200
H	-3.67601800	-2.04373900	-0.18561400
H	-3.73178700	-1.55681100	1.51447000
H	-6.02584300	-2.12008500	0.67626200
H	-5.66030100	-1.54197500	-1.72966400
H	-7.07016500	-0.68591400	-1.10257700
H	6.61146100	3.95806100	-1.05066100
H	5.70421100	2.85732500	-2.12293900
H	6.35270700	2.26104600	-0.56148100
C	0.84767000	-2.70333100	-1.42762000
H	-0.01778900	-3.24862400	-1.06077800
C	1.42825200	-3.20347800	-2.63200500
N	1.88801600	-3.61642800	-3.62016400

<b>DFT Theory Level</b>	B3LYP/6-311G++(d,p)
<b>Energy (Hartree)</b>	-1495.468935



Cartesian coordinates of optimized enediyne **33** at B3LYP/6-311G++(d,p) level of theory, in gas phase.

C	3.12306000	-1.90209000	3.46997500
C	4.34014300	-2.08107000	2.89181200
C	2.01664000	-1.60236600	2.63824900
C	4.45741000	-1.95885900	1.48642500
C	4.25378300	-1.79834000	0.30561500
C	3.84517500	-1.58117200	-1.07322700
C	2.48553300	-0.80391400	-1.22154000
C	1.28176300	-1.35867700	1.71039400
C	1.44561100	2.43833600	0.54783900
C	2.56543300	3.22574400	0.36966700
C	3.67837300	2.71268400	-0.30667600

C	3.64655100	1.40854000	-0.79065700
C	2.51030900	0.60144500	-0.62249800
C	1.39997700	1.13166900	0.04242200
N	0.25063300	0.30730900	0.25050500
C	0.53096000	-1.12184000	0.47576000
C	1.29549800	-1.62374200	-0.74795400
C	-1.03442200	0.78999600	0.04521600
O	-1.95042900	-0.17831800	0.26659400
O	-1.28268000	1.93081000	-0.27788500
C	-5.31508200	0.58552800	-1.38988400
C	-5.79752600	1.67244300	-0.40762400
C	-5.40701800	1.27978900	1.03166000
C	-3.86911800	1.15819800	1.12896400
C	-3.39511400	0.08293100	0.13851900
C	-3.77670700	0.46232900	-1.30042400
C	-6.05915600	-0.06853300	1.39339000
C	-4.03485300	-1.26534400	0.50190000
C	-5.57014800	-1.15161600	0.41133100
C	-5.96715500	-0.76288200	-1.02614900
O	4.74142300	3.55984000	-0.43216700
C	5.90775200	3.09854900	-1.09916500
H	3.00098900	-1.98979400	4.54323200
H	5.20742700	-2.31462500	3.49921800
H	4.61919300	-1.03784000	-1.62227600
H	3.74565100	-2.54230600	-1.58614500
H	2.35894800	-0.68907200	-2.30568500
H	0.58573000	2.83405400	1.06837100
H	2.60439700	4.23784800	0.75291200
H	4.50661000	1.00764600	-1.30684100
H	-0.42634300	-1.63371000	0.52501600
H	-5.58742100	0.86514600	-2.41261500
H	-6.88456500	1.78938300	-0.48226400
H	-5.35189100	2.63876400	-0.66750000
H	-5.74374000	2.05330200	1.72934800
H	-3.39556000	2.11283100	0.89788000
H	-3.57198700	0.87122700	2.14373900
H	-3.41511300	-0.31145100	-1.98675200
H	-3.29975100	1.40378900	-1.57584300
H	-7.15084300	0.01503200	1.34715700
H	-5.80351900	-0.34838500	2.42187500
H	-3.66685200	-2.03621400	-0.18358100
H	-3.72746700	-1.55031000	1.51337400
H	-6.01541500	-2.11740300	0.67148700
H	-5.64704200	-1.53965500	-1.73009900
H	-7.05743100	-0.68849200	-1.10749800
H	6.61156000	3.92888800	-1.07586900
H	5.69546400	2.83471300	-2.14126100
H	6.34816300	2.23672200	-0.58566300
C	0.83176900	-2.70331300	-1.40132700
H	-0.02961800	-3.24562300	-1.02619900

C            1.40060300 -3.20800800 -2.60426500  
 N            1.84703200 -3.62468100 -3.58712400

### 3. Comparative table on the important structural parameters of the theoretical models with the available crystal data for compound 17 and 29

#### Compound 17

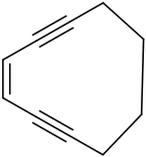
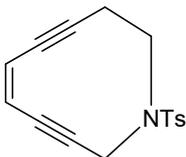
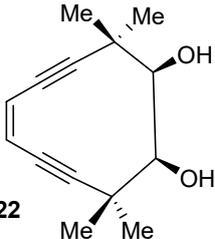
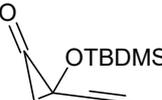
Model	a-b (distance in Å)	c-d (distance in Å)	Bond angle (in degrees)				RMSD (in Å)  (obtained using VMD software)
			P <sub>a</sub>	P <sub>b</sub>	P <sub>c</sub>	P <sub>d</sub>	
Crystal	2.778	3.661	172.61	169.44	173.15	170.50	Reference
Optimized Model from 6-31G+(d,p)	2.834	3.763	171.88	170.56	172.24	169.24	0.1288
Optimized Model from 6- 311G++(d,p)	2.829	3.748	171.76	170.29	172.47	169.56	0.1243

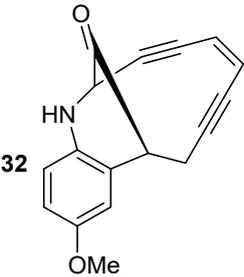
#### Compound 29

Model	a-b (distance in Å)	c-d (distance in Å)	Bond angle (in degrees)				RMSD (in Å)  (obtained using VMD software)
			P <sub>a</sub>	P <sub>b</sub>	P <sub>c</sub>	P <sub>d</sub>	
Crystal	2.720	3.391	168.66	165.71	171.57	169.81	Reference
Optimized Model from 6-31G+(d,p)	2.748	3.418	168.62	164.93	172.52	170.90	0.2033

Optimized Model from 6- 311G++(d,p)	2.740	3.414	168.71	165.29	172.39	170.59	0.2117
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**4. Comparative table on the important structural parameters and energy values for some of the borderline compounds (with respect to the average interior angle value) using B3LYP/6-311G(d,p) along with the previously used theory levels**

Molecular Structure with ID	Theory Level	cd-distance (in Å)	P <sub>a</sub> (in degree)	P <sub>b</sub> (in degree)	(P <sub>a</sub> +P <sub>b</sub> )/2 (in degree)	Energy (Hartree)
 <b>14</b>	B3LYP/6-311G++(d,p)	3.383	165.89	165.89	165.89	-387.045722
	B3LYP/6-31G+ (d,p)	3.376	165.40	165.40	165.40	-386.969326
	B3LYP/6-311G(d,p)	3.389	166.00	166.00	166.00	-387.042017
 <b>19</b>	B3LYP/6-311G++(d,p)	3.338	164.72	166.53	165.63	-1222.152364
	B3LYP/6-31G+ (d,p)	3.339	164.24	166.38	165.31	-1221.957159
	B3LYP/6-311G(d,p)	3.340	164.68	166.56	165.62	-1222.140738
 <b>22</b>	B3LYP/6-311G++(d,p)	3.436	166.60	166.43	166.52	-694.813768
	B3LYP/6-31G+ (d,p)	3.441	166.33	166.25	166.29	-694.665975
	B3LYP/6-311G(d,p)	3.452	166.99	166.39	166.69	-694.803080
 <b>30</b>	B3LYP/6-311G++(d,p)	3.456	168.73	166.87	167.80	-1140.495397
	B3LYP/6-	3.468	168.99	166.68	167.84	-1140.296648

	31G+ (d,p)					
	B3LYP/6-311G(d,p)	3.457	168.59	166.95	167.77	-1140.487140
 <p>32</p>	B3LYP/6-311G++(d,p)	3.416	167.22	166.73	166.98	-860.896923
	B3LYP/6-31G+ (d,p)	3.420	167.17	166.49	166.83	-860.718146
	B3LYP/6-311G(d,p)	3.422	167.21	166.84	167.03	-860.882651